

ACCELERATING APACHE SPARK 3.X

Leveraging NVIDIA GPUs
to Power the Next Era
of Analytics and AI

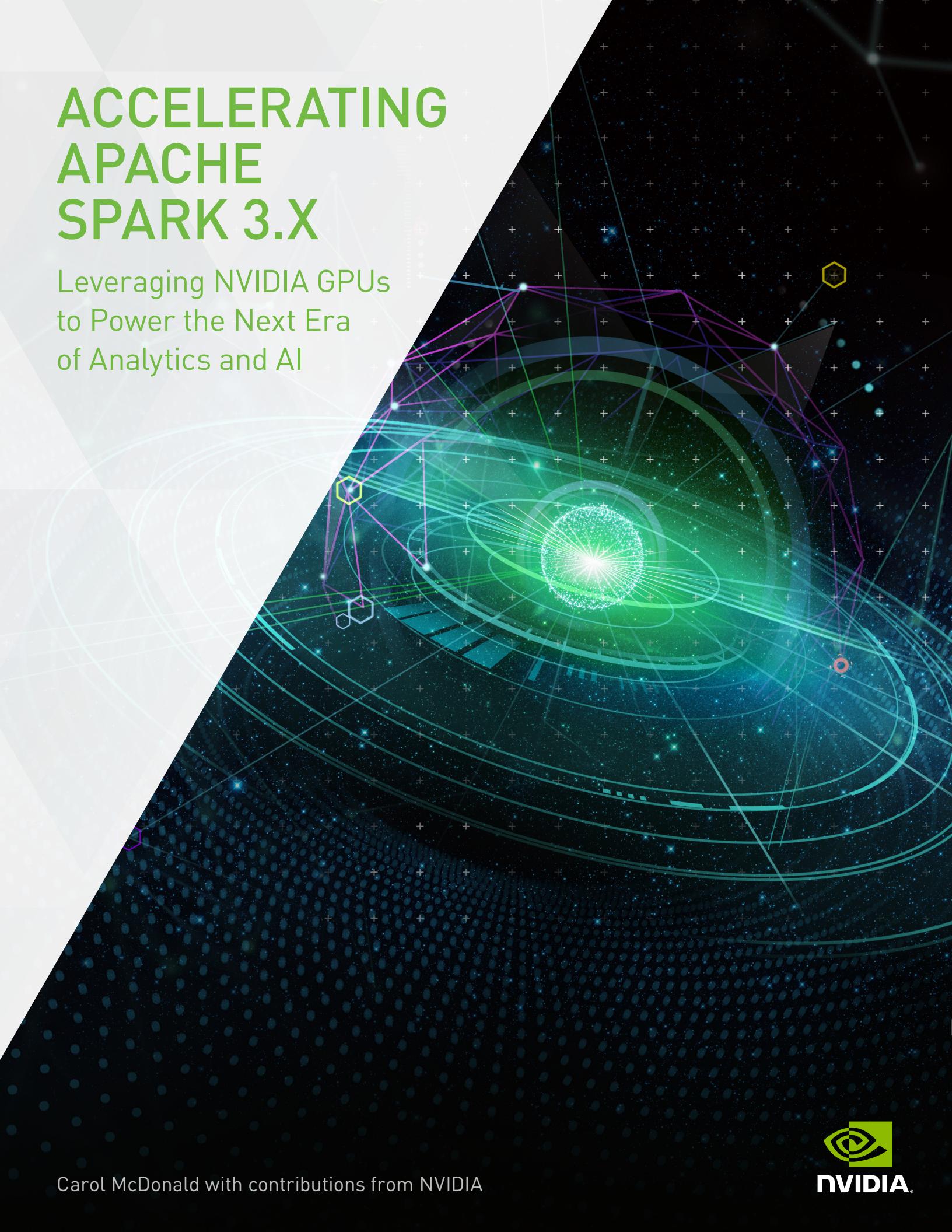


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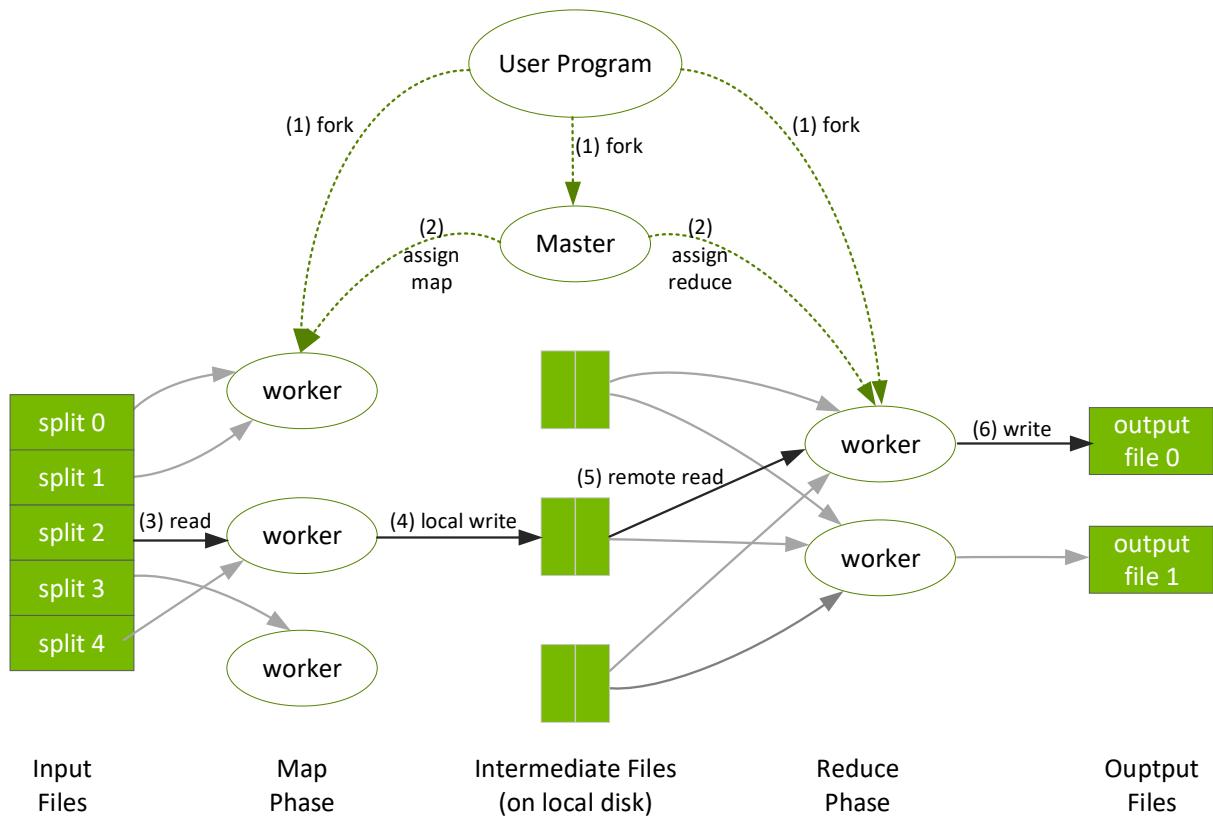
Preface: Why are GPUs Driving the Next Wave of Data Science?

The Evolution of Data Analytics

According to Thomas Davenport in the updated version of Competing on Analytics, analytical technology has changed dramatically over the last decade, with more powerful and less expensive distributed computing across commodity servers, and improved machine learning (ML) technologies, enabling companies to store and analyze many different types of data and far more of it.

The Beginning of Big Data Processing

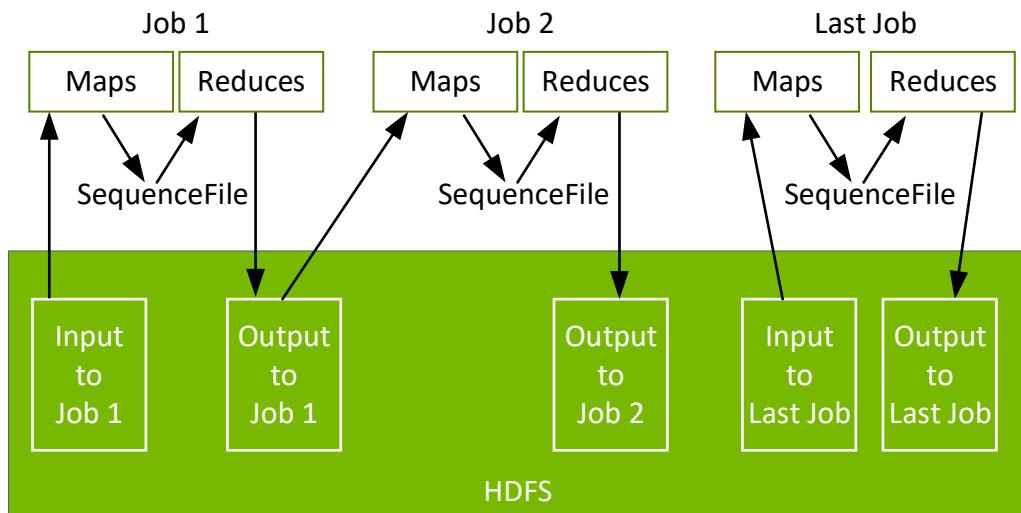
Google invented a distributed file system and MapReduce, a resilient distributed processing framework, in order to index the exploding volume of content on the web, across large clusters of commodity servers. The Google file system (GFS) partitioned, distributed, and replicated file data across the data nodes in a cluster. MapReduce distributed computation across the data nodes in a cluster: users specify a map function that processes a key/value pair to generate a set of intermediate key/value pairs and a reduce function that merges all intermediate values associated with the same intermediate key. Both the GFS and MapReduce were designed for fault tolerance by failing over to another node for data or processing.



Reference: [MapReduce Google White Paper](#)

A year after Google published a [white paper describing the MapReduce framework](#), Doug Cutting and Mike Cafarella created [Apache Hadoop™](#).

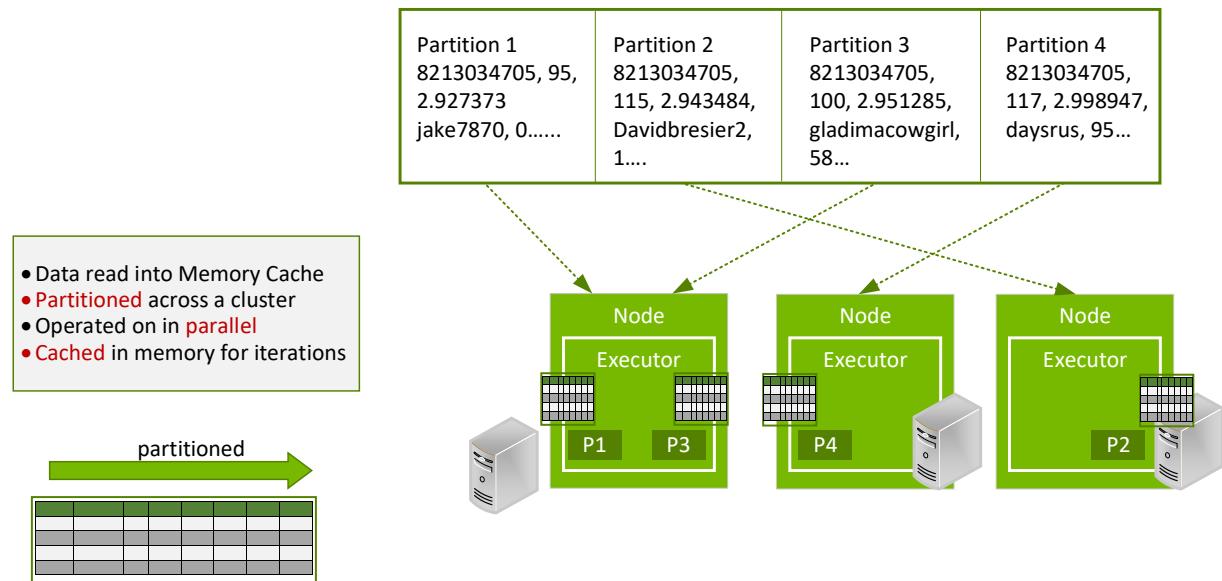
However, Hadoop performance is bottlenecked by its model of checkpointing results to disk. At the same time, Hadoop adoption has been hindered by the low-level programming model of MapReduce. Data pipelines and iterative algorithms require chaining multiple MapReduce jobs together, which can be difficult to program and cause a lot of reading and writing to disk.



Apache Spark Makes Big Data Processing Faster and Easier

Apache Spark started as a [research project](#) at UC Berkeley in the AMPLab, became a top level [Apache Software Foundation](#) project in 2014, and is now maintained by a community of hundreds of developers from hundreds of organizations. Spark was developed with the goal of keeping the benefits of MapReduce's scalable, distributed, fault-tolerant processing framework, while making it more efficient and easier to use. Spark is more efficient than MapReduce for data pipelines and iterative algorithms because it caches data in memory across iterations and uses lighter weight threads. Spark also provides a richer functional programming model than MapReduce.

Distributed Datasheet

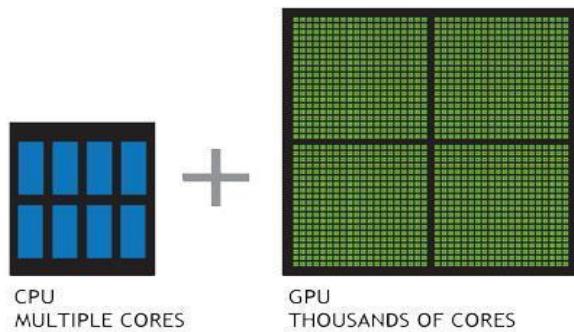


Spark mitigated the I/O problems found in Hadoop, but now the bottleneck has shifted from I/O to compute for a growing number of applications. This performance bottleneck has been thwarted with the advent of GPU-accelerated computation.

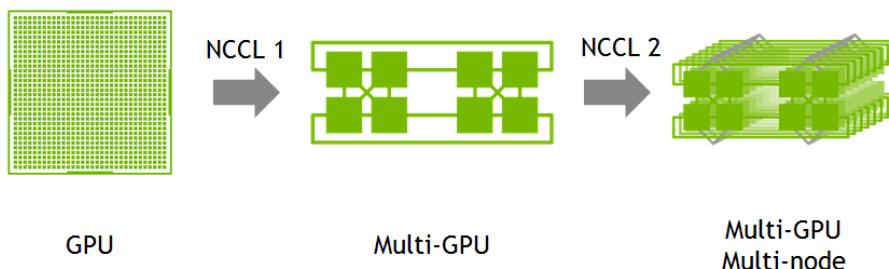
GPUs Accelerate Computer Processing

Graphics Processing Units (GPUs) are popular for their extraordinarily low price per flop (performance) and are addressing the compute performance bottleneck today by speeding up multi-core servers for parallel processing.

A CPU consists of a few cores, optimized for sequential serial processing. Whereas, a GPU has a massively parallel architecture consisting of thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously. GPUs are capable of processing data much faster than configurations containing CPUs alone.



Once large amounts of data need to be broadcasted, aggregated, or collected across nodes in a cluster, the network can become a bottleneck. [GPUDirect Remote](#) direct memory access with the [NVIDIA Collective Communications Library](#) can solve this bottleneck by allowing GPUs to communicate directly with each other, across nodes, for faster multi-GPU and multi-node reduction operations.



The benefits of GPUDirect RDMA are also critical for large, complex extract, transform, load (ETL) workloads, allowing them to operate as if they were on one massive server.

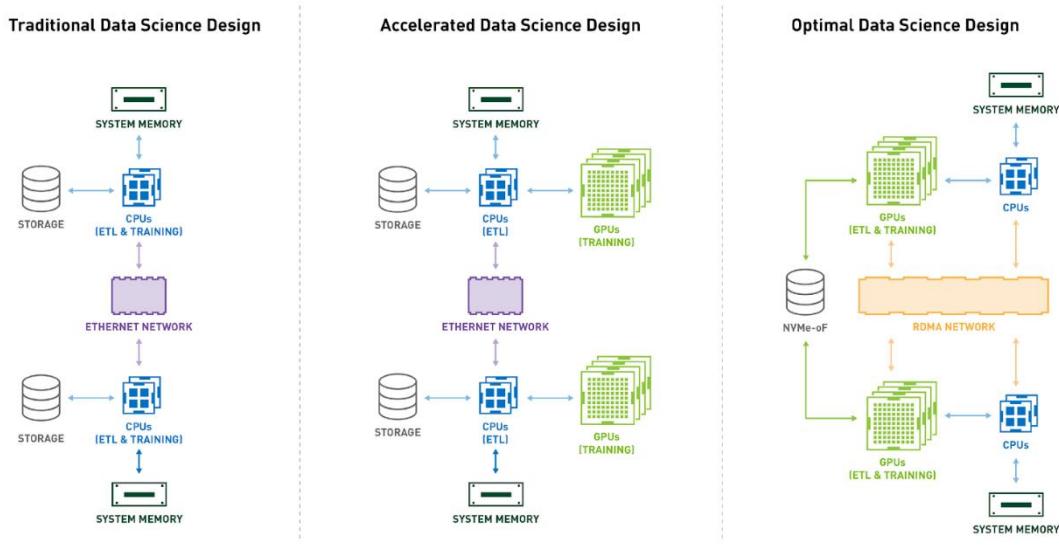


FIGURE 2: MOVING TO A GPU-CENTRIC DATA SCIENCE DESIGN

GPU-Accelerated Data Science Powered by RAPIDS

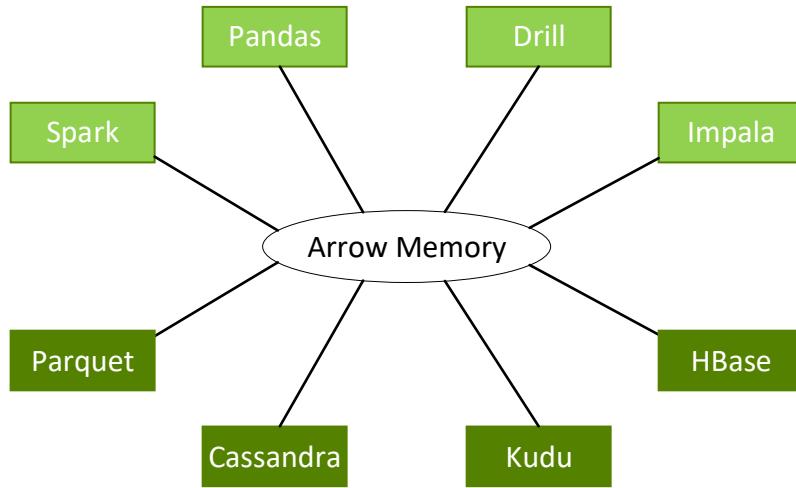
A key component of data science is data exploration. Preparing a data set for ML requires understanding the data set, cleaning and manipulating data types and formats, and extracting features for the learning algorithm. These tasks are grouped under the term ETL. ETL is often an iterative, exploratory process. As data sets grow, the interactivity of this process suffers when running on CPUs.

GPUs have been responsible for the advancement of deep learning (DL) in the past several years, while ETL and traditional ML workloads continued to be written in Python, often with single-threaded tools like Scikit-Learn or large, multi-CPU distributed solutions like Spark.

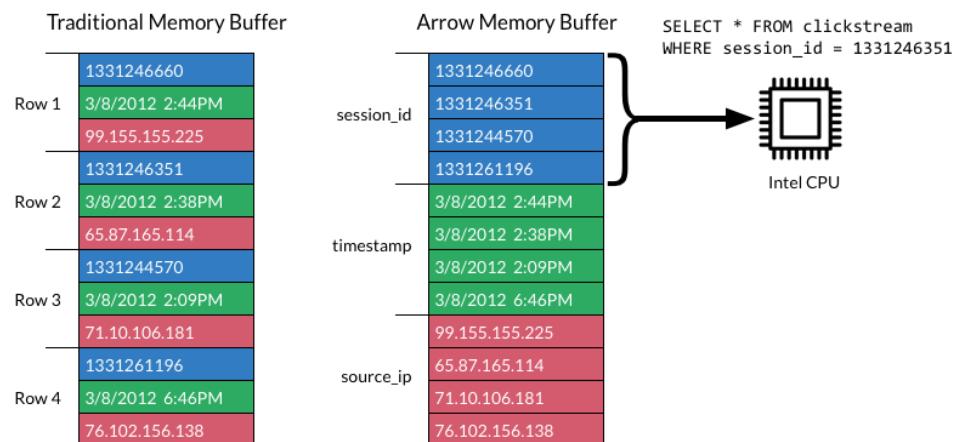
RAPIDS is a suite of open-source software libraries and APIs for executing end-to-end data science and analytics pipelines entirely on GPUs, achieving speedup factors of 50X or more on typical end-to-end data science workflows. RAPIDS accelerates the entire data science pipeline, including data loading, enabling more productive, interactive, and exploratory workflows.

Built on top of NVIDIA® CUDA®, an architecture and software platform for GPU computing, RAPIDS exposes GPU parallelism and high-bandwidth memory speed through user-friendly APIs. RAPIDS focuses on common data preparation tasks for analytics and data science, offering a powerful GPU DataFrame that is compatible with ApacheArrow data structures with a familiar DataFrame API.

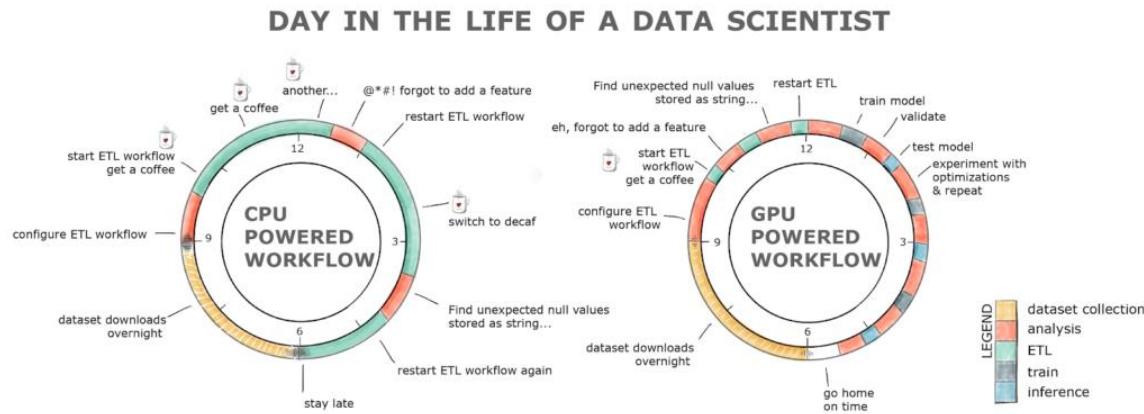
Apache Arrow specifies a standardized language-independent columnar memory format, optimized for data locality, to accelerate analytical processing performance on modern CPUs or GPUs, and provides zero-copy streaming messaging and interprocess communication without serialization overhead.



	session_id	timestamp	source_ip
Row 1	1331246660	3/8/2012 2:44PM	99.155.155.225
Row 2	1331246351	3/8/2012 2:38PM	65.87.165.114
Row 3	1331244570	3/8/2012 2:09PM	71.10.106.181
Row 4	1331261196	3/8/2012 6:46PM	76.102.156.138



The DataFrame API integrates with a variety of ML algorithms without incurring typical serialization and deserialization costs, enabling end-to-end pipeline accelerations.



By hiding the complexities of low-level CUDA programming, RAPIDS creates a simple way to execute data science tasks. As more data scientists use Python and other high-level languages, providing acceleration with minimal to no code change is essential to rapidly improving development time.

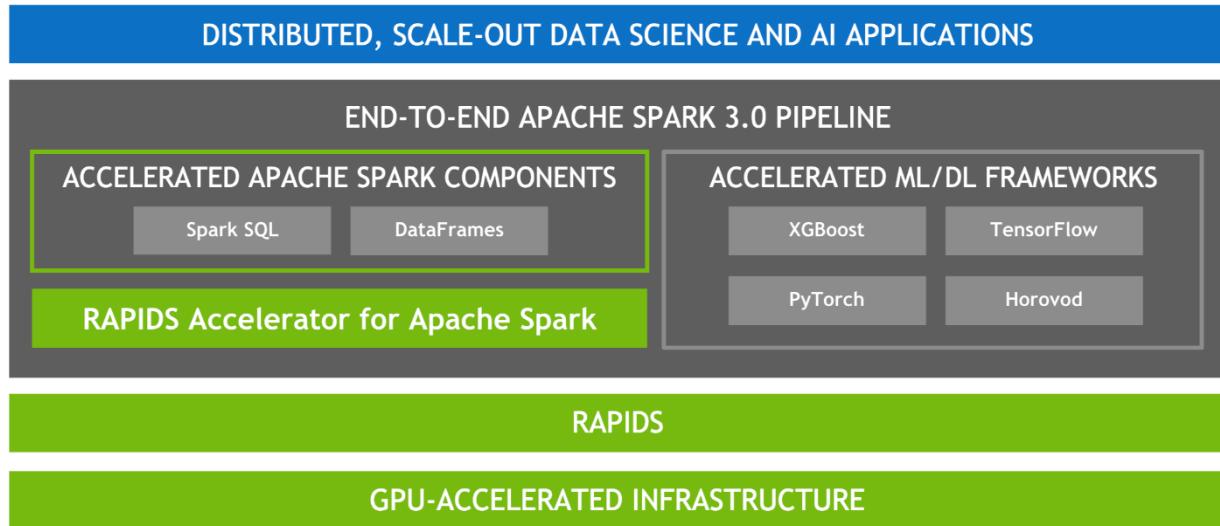
Boosting Data Science Frameworks with GPUs and the RAPIDS Library

Another way RAPIDS accelerates development is with integration to leading data science frameworks, such as [PyTorch](#), [Chainer](#), and [ApacheMxNet](#) for DL and distributed computing frameworks like [Apache Spark](#) and [Dask](#) for seamless scaling from GPU workstations to multi-GPU servers and multi-node clusters. Also, products such as [BlazingSQL](#), an open source SQL engine, are being built on top of RAPIDS, adding even more accelerated capabilities for users.

Apache Spark 3.x empowers GPU applications by providing user APIs and configurations to easily request and utilize GPUs and is now extensible to allow columnar processing on the GPU; all of which wasn't supported prior to Spark 3.x. Internally, Spark added GPU scheduling, further integration with the cluster managers (YARN, Kubernetes, etc.) to request GPUs, and plugin points to allow it to be extended to run operations on the GPU. This makes GPUs easier to request and use for Spark application developers, allows for closer integration with DL and AI frameworks, such as Horovod and TensorFlow on Spark, and allows for better utilization of GPUs. This extensibility also allows columnar processing, which opens up the possibility for users to add plugins that accelerate queries using the GPU.

Later in this eBook, we explore how the Apache Spark 3.x stack shown below accelerates Spark 3.x applications.

APACHE SPARK 3.x GPU-ACCELERATED SOFTWARE STACK



NVIDIA GPUs in Action

Regardless of industry or use case, when putting ML into action, many data science problems break down into similar steps: iteratively preprocessing data to build features, training models with different parameters, and evaluating the model to ensure performance translates into valuable results.

RAPIDS helps accelerate all of these steps while maximizing the user's hardware investments. Early customers have taken full data pipelines that took days, if not weeks, and ran them in minutes. They've simultaneously reduced costs and improved the accuracy of their models since more iterations allow data scientists to explore more models and parameter combinations, as well as train on larger datasets.

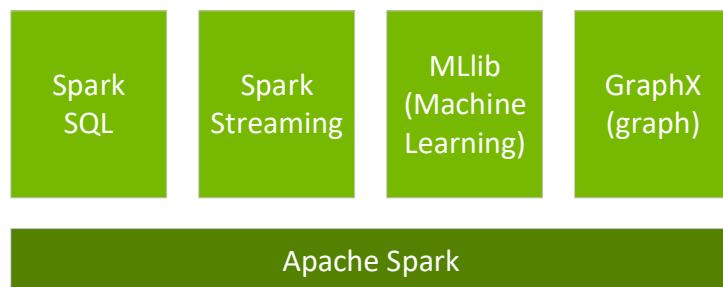
Retailers are improving their forecasting. Finance companies are getting better at assessing credit risk. And adtech firms are enhancing their ability to predict click-through rates. Data scientists often achieve improvements of 1-2 percent. This can translate to tens or hundreds of millions of dollars of revenue and profitability.

Chapter 1: Introduction to Spark Processing

[IDC predicts](#) that data generated in data centers, as well as from edge computing and IOT, will quintuple in the next seven years to 175 ZB. In tandem with the monumental growth of data, Apache Spark from Apache Software Foundation has become one of the most popular frameworks for distributed scale-out data processing, running on millions of servers—both on premises and in the cloud. This chapter provides an introduction to the Spark framework and explains how it executes applications.

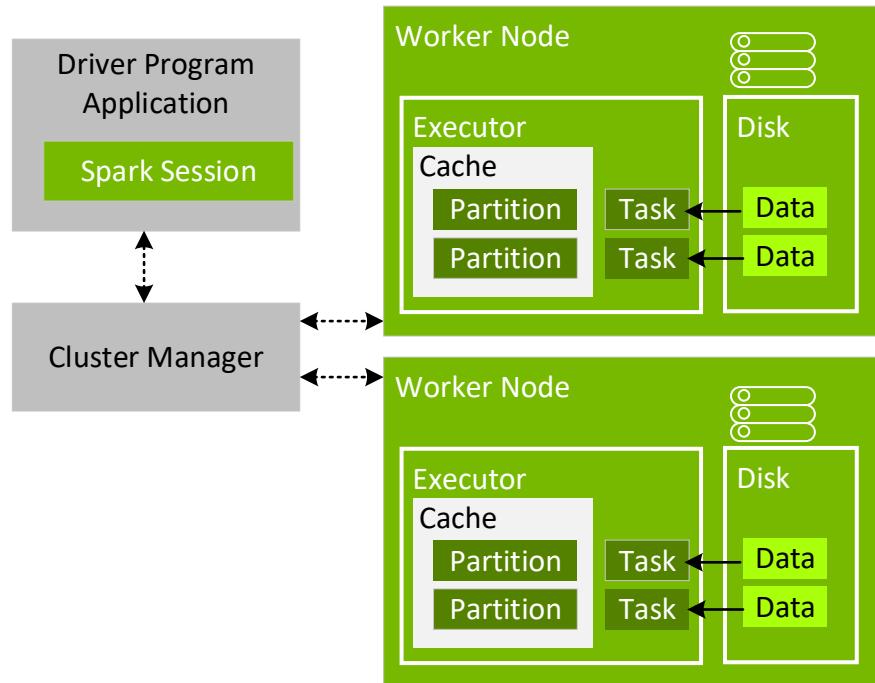
Apache Spark is a fast and general purpose analytics engine for large-scale data processing, that runs on Hadoop, Apache Mesos, Kubernetes, standalone, or in the cloud. Spark offers high-level operators that make it easy to build parallel applications in Scala, Python, R, or SQL, using an interactive shell, notebooks, or packaged applications.

On top of the Spark core data processing engine, there exist libraries for SQL and DataFrames, machine learning, GraphX, graph computation, and stream processing. These libraries can be used together on massive datasets from a variety of data sources, such as HDFS, Alluxio, Apache Cassandra, Apache HBase, or Apache Hive.



How Spark Executes on a Cluster

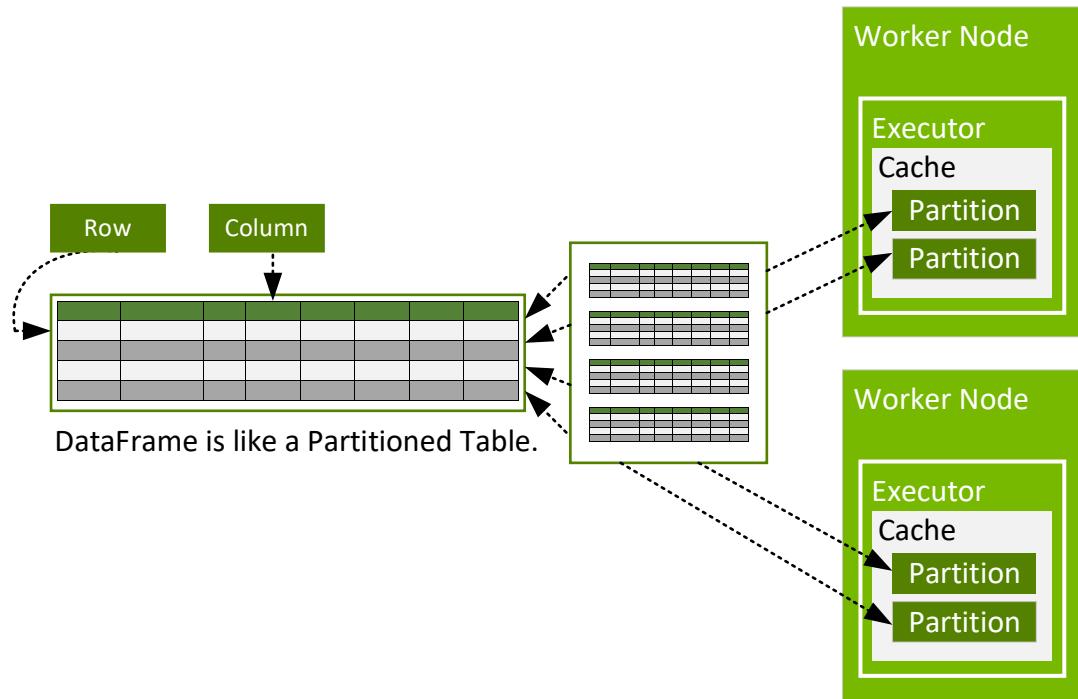
A Spark application runs as parallel tasks inside of executor processes on cluster nodes, with execution coordinated between the `SparkSession` object in the driver program and the Resource or Cluster manager (either Standalone, Mesos, YARN, or Kubernetes) on the cluster.



Spark can also run on a single machine, called local mode. In local mode, the driver program and the tasks run in threads in the same Java Virtual Machine. Local mode is useful for prototyping, development, debugging and testing. However local mode is not meant for running production applications.

Creating a DataFrame from a File

A Spark DataFrame is a distributed `Dataset` of `org.apache.spark.sql.Row` objects, that are partitioned across multiple nodes in a cluster and can be operated on in parallel. A DataFrame represents a table of data with rows and columns, similar to a DataFrame in R or Python, but with Spark optimizations. A DataFrame consists of partitions, each of which is a range of rows in cache on a data node.



DataFrames can be constructed from data sources, such as csv, parquet, JSON files, Hive tables, or external databases. A DataFrame can be operated on using relational transformations and Spark SQL queries.

The Spark shell or Spark notebooks provide a simple way to use Spark interactively. You can start the shell in local mode with the following command:

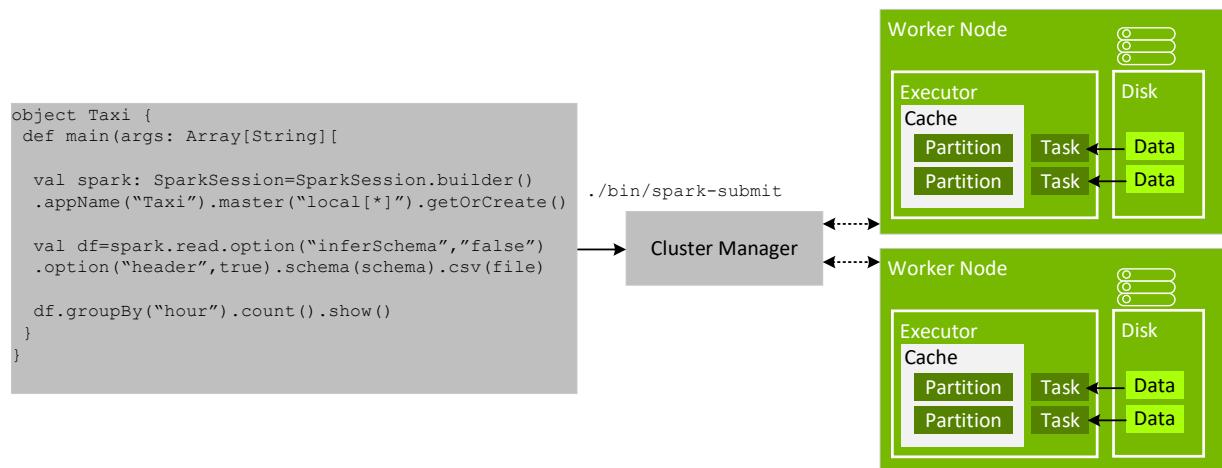
```
$ /[installation path]/bin/spark-shell --master local[2]
```

You can then enter the code from the rest of this chapter into the shell to see the results interactively. In the code examples, the outputs from the shell are prefaced with the result.

For execution coordination between your application driver and the Cluster manager, you create a `SparkSession` object in your program, as shown in the following code example:

```
val spark = SparkSession.builder.appName("Simple Application").master("local[2]").getOrCreate()
```

When a Spark application starts, it connects to the cluster manager via the master URL. The master URL can be set to the cluster manager or local[N] to run locally with N threads, when creating the SparkSession object or when submitting the Spark application. When using the spark-shell or notebook, the SparkSession object is already created and available as the variable spark. Once connected, the cluster manager allocates resources and launches executor processes, as configured for the nodes in your cluster. When a Spark application executes, the SparkSession sends tasks to the executors to run.



With the SparkSession read method, you can read data from a file into a DataFrame, specifying the file type, file path, and input options for the schema.

```

import org.apache.spark.sql.types._
import org.apache.spark.sql._
import org.apache.spark.sql.functions._

val schema =
  StructType(Array(
    StructField("vendor_id", DoubleType),
    StructField("passenger_count", DoubleType),
    StructField("trip_distance", DoubleType),
    StructField("pickup_longitude", DoubleType),
    StructField("pickup_latitude", DoubleType),
    StructField("rate_code", DoubleType),
    StructField("store_and_fwd", DoubleType),
    StructField("dropoff_longitude", DoubleType),
    StructField("dropoff_latitude", DoubleType),
    StructField("fare_amount", DoubleType),
    StructField("hour", DoubleType),
    StructField("year", IntegerType),
    StructField("month", IntegerType),
    StructField("day", DoubleType),
    StructField("day_of_week", DoubleType),
  ))

```

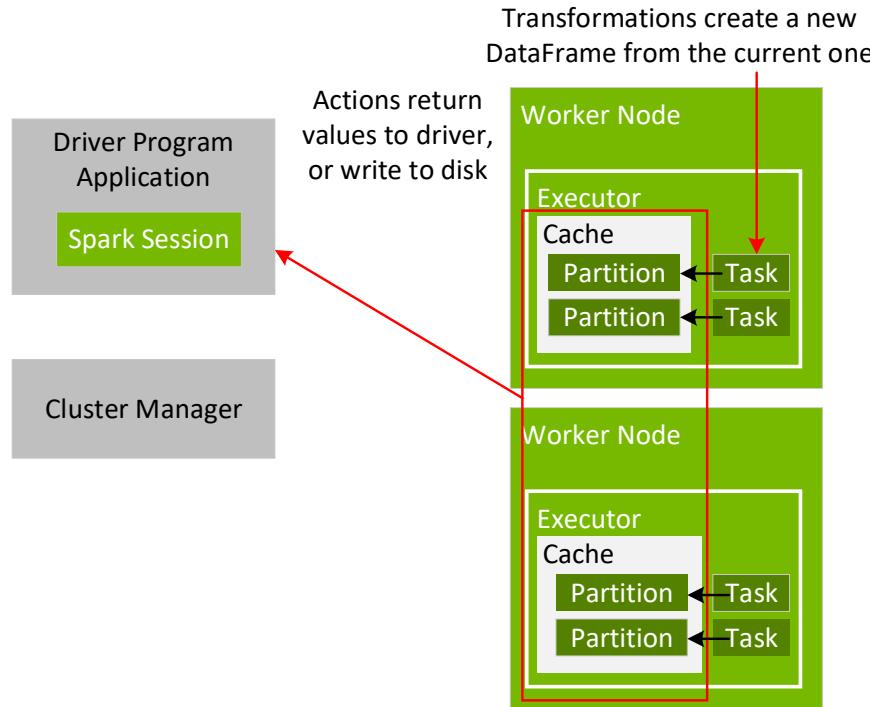
```
    StructField("is_weekend", DoubleType)
  ))  
  
val file = "/data/taxi_small.csv"  
  
val df = spark.read.option("inferSchema", "false")  
.option("header", true).schema(schema).csv(file)  
  
result:  
df: org.apache.spark.sql.DataFrame = [vendor_id: double, passenger_count:  
double ... 14 more fields]
```

The take method returns an array with objects from this DataFrame, which we see is of the `org.apache.spark.sql.Row` type.

```
df.take(1)  
result:  
Array[org.apache.spark.sql.Row] = Array([4.52563162E8,5.0,2.72,-  
73.948132,40.82982699999995,-6.77418915E8,-1.0,-  
73.969648,40.79747200000006,11.5,10.0,2012,11,13.0,6.0,1.0])
```

DataFrame Transformations and Actions

DataFrames provide a domain-specific language API for structured data processing, known as transformations. Transformations create a new transformed DataFrame from the current DataFrame and are lazily evaluated. Transformations are executed when triggered by an action, which returns a result to the driver program or writes to disk. Once an action has run and the value is returned, the DataFrame is no longer in memory, unless it is cached. Spark can cache DataFrames using an in-memory columnar format by calling [`dataFrame.cache\(\)`](#).



Here is a list of some commonly used DataFrame transformations.

- ▶ `select` Selects a set of columns
- ▶ `join` Join with another DataFrame, using the given join expression
- ▶ `groupBy` Groups the DataFrame, using the specified columns

This `groupBy` transformation example groups the taxi DataFrame by hour of the day, then the `count` action totals the number of taxi trips for each hour. The `show` action prints out the resulting DataFrame rows in a tabular format.

```
df.groupBy("hour").count().show(4)

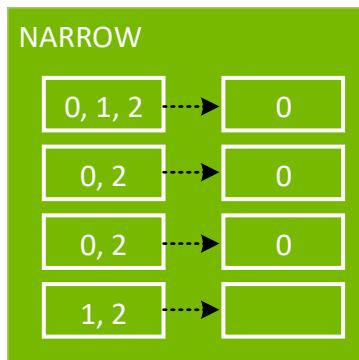
result:
+----+---+
|hour|count|
+----+---+
| 0.0|   12|
| 1.0|   49|
| 2.0|  658|
| 3.0|  742|
+----+---+
```

Following is a list of some commonly used DataFrame actions.

- ▶ `show(n)` Displays the first n rows in a tabular format
- ▶ `take(n)` Returns the first n rows in the DataFrame in an array
- ▶ `count` Returns the number of rows in the DataFrame

DataFrame Transformation Narrow and Wide Dependencies

There are two types of DataFrame transformations, those with narrow dependencies and those with wide dependencies. Transformations with narrow dependencies do not have to move data between partitions when creating a new DataFrame from an existing one. An example narrow transformation is `filter()` which is used to filter the rows from a DataFrame based on the given SQL expression. The following example filters for the hour value = 0.

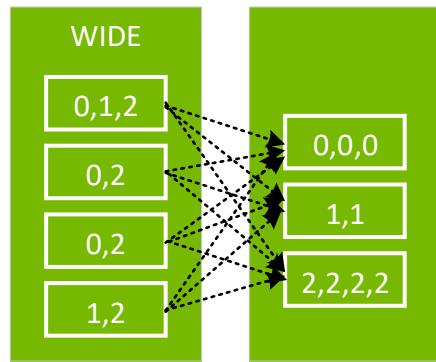


Multiple narrow transformations can be performed on a DataFrame in memory, using a process called pipelining, making narrow transformations very efficient. Narrow transformations like `filter` and `select` are used in the example below to retrieve taxi fare_amounts for the 0 hour of the day.

```
// select and filter are narrow transformations
df.select($"hour", $"fare_amount").filter($"hour" === "0.0" ).show(2)

result:
+---+-----+
|hour|fare_amount|
+---+-----+
| 0.0|      10.5|
| 0.0|      12.5|
+---+-----+
```

Transformations with wide dependencies have to move data between partitions, when creating a new DataFrame from an existing one, in a process called a shuffle. Shuffles send data across the network to other nodes and write to disk, causing network and disk I/O. Example wide transformations are `groupBy`, `agg`, `sortBy`, and `orderBy`. The wide transformation shows groups by the hour value.



Following is a wide transformation to group by the hour value and count the number of taxi trips by hour.

```
df.groupBy("hour").count().show(4)
```

```
result:
+----+---+
|hour|count|
+----+---+
| 0.0|   12|
| 1.0|   49|
| 2.0|  658|
| 3.0|  742|
+----+---+
```

How a Spark Application Executes

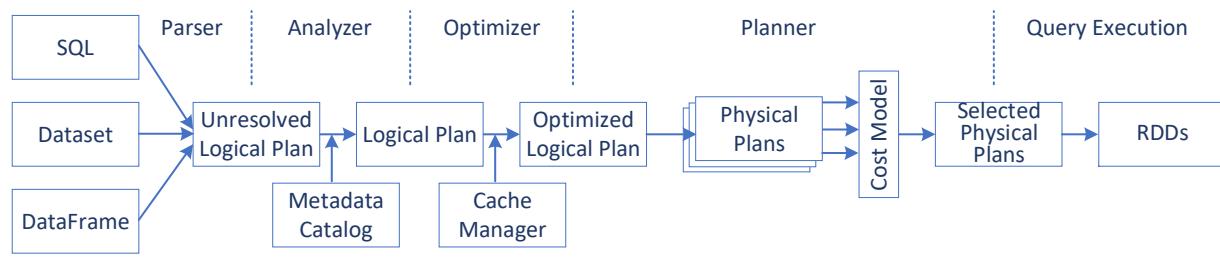
When a Spark query executes, it goes through the following steps:

- ▶ Creates a logical plan
- ▶ Transforms the logical plan to a physical plan
- ▶ Generates code
- ▶ Executes the tasks on a cluster

Apache Spark provides a web UI that you can use to see a visual representation of these plans in the form of Directed Acyclic Graphs (DAGs). With the web UI, you can also see how the plan executes and monitor the status and resource consumption on your Spark cluster. You can view the web UI in real time with this URL: <http://<driver-node>:4040>. You can view the web UI after execution through Spark's history server at <http://<server-url>:18080>, provided that the application's event logs exist.

In the first step, the logical plan is created for the submitted SQL or DataFrame. The logical plan shows the set of abstract transformations that will be executed. The Spark Analyzer uses the Metadata Catalog to resolve tables and columns, then passes the plan to the [Catalyst Optimizer](#), which uses rules like **filter push down**, to optimize the plan.

Actions trigger the translation of the logical DAG into a physical execution plan. The physical plan identifies resources that will execute the plan, using a cost model for different execution strategies. An example of this would be a **broadcast join** versus a **hash join**.



Reference: Databricks

Viewing the Physical Plan

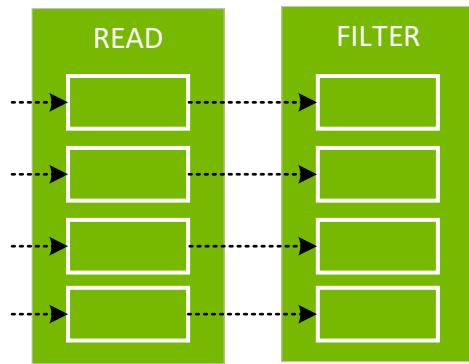
You can see the formatted physical plan for a DataFrame by calling the `explain("formatted")` method. In the physical plan below, the DAG for `df2` consists of a Scan `csv` file, a Filter on `day_of_week`, and a Project (selecting columns) on `hour`, `fare_amount`, and `day_of_week`.

```
val df = spark.read.option("inferSchema", "false") .option("header",
true).schema(schema).csv(file)
val df2 = df.select($"hour", $"fare_amount",
$"day_of_week").filter($"day_of_week" === "6.0" )
df2.show(3)
result:
+---+-----+
|hour|fare_amount|day_of_week|
+---+-----+
|10.0|      11.5|       6.0|
|10.0|      5.5|       6.0|
|10.0|     13.0|       6.0|
+---+-----+
df2.explain("formatted")
result:
== Physical Plan ==
* Project (3)
+- * Filter (2)
  +- Scan csv  (1)

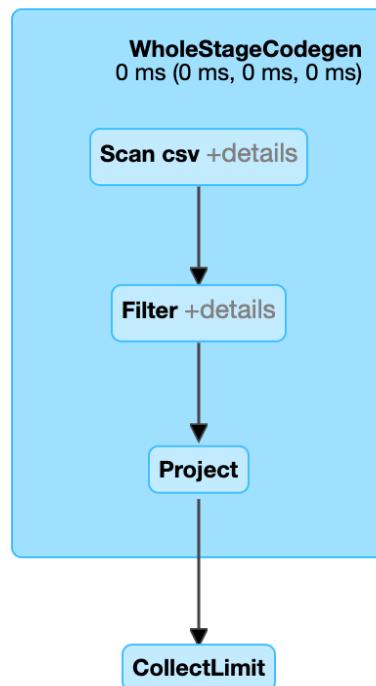
(1) Scan csv
Location: [dbfs:/FileStore/tables/taxi_tsmall.csv]
Output [3]: [fare_amount#143, hour#144, day_of_week#148]
PushedFilters: [IsNotNull(day_of_week), EqualTo(day_of_week, 6.0) ]

(2) Filter [codegen id : 1]
Input [3]: [fare_amount#143, hour#144, day_of_week#148]
Condition : (isnotnull(day_of_week#148) AND (day_of_week#148 = 6.0))

(3) Project [codegen id : 1]
Output [3]: [hour#144, fare_amount#143, day_of_week#148]
Input [3]: [fare_amount#143, hour#144, day_of_week#148]
```



You can see more details about the plan produced by Catalyst on the web UI SQL tab. Clicking on the query description link displays the DAG and details for the query.



In the following code, after the explain, we see that the physical plan for df3 consists of a Scan, Filter, Project, HashAggregate, Exchange, and HashAggregate. The Exchange is the shuffle caused by the groupBy transformation. Spark performs a hash aggregation for each partition before shuffling the data in the Exchange. After the exchange, there is a hash aggregation of the previous sub-aggregations. Note that we would have an in-memory scan instead of a file scan in this DAG, if df2 were cached.

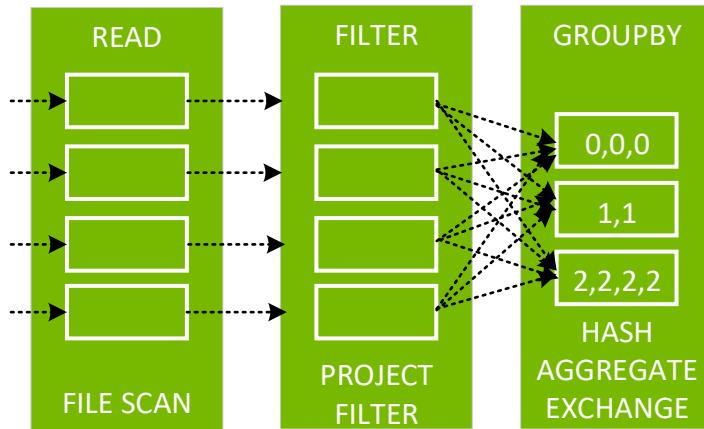
```

val df3 = df2.groupBy("hour").count
df3.orderBy(asc("hour")) show(5)
result:
+----+---+
|hour|count|
+----+---+
| 0.0|   12|
| 1.0|   47|
| 2.0|  658|
| 3.0|  742|
| 4.0|  812|
+----+---+

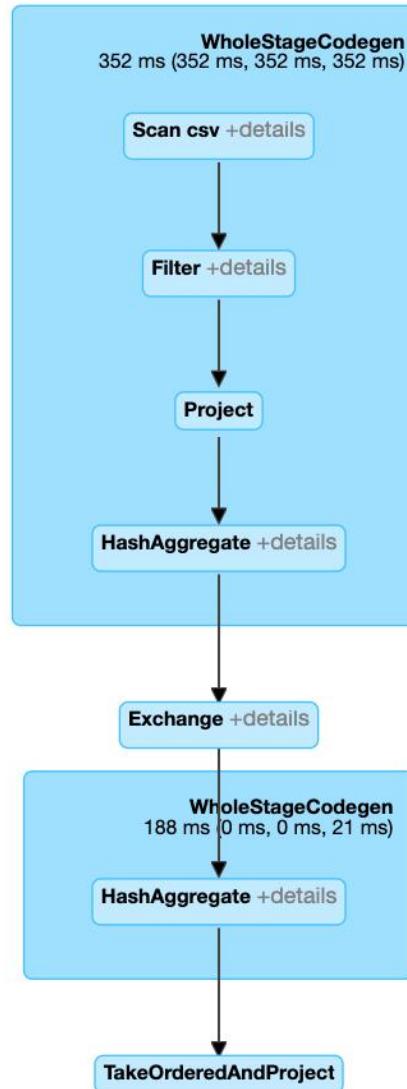
df3.explain
result:
== Physical Plan ==
* HashAggregate (6)
+- Exchange (5)
  +- * HashAggregate (4)
    +- * Project (3)
      +- * Filter (2)
        +- Scan csv  (1)
(1) Scan csv
Output [2]: [hour, day_of_week]
(2) Filter [codegen id : 1]
Input [2]: [hour, day_of_week]
Condition : (isnotnull(day_of_week) AND (day_of_week = 6.0))
(3) Project [codegen id : 1]
Output [1]: [hour]
Input [2]: [hour, day_of_week]
(4) HashAggregate [codegen id : 1]
Input [1]: [hour]
Functions [1]: [partial_count(1) AS count]
Aggregate Attributes [1]: [count]
Results [2]: [hour, count]
(5) Exchange
Input [2]: [hour, count]
Arguments: hashpartitioning(hour, 200), true, [id=]
(6) HashAggregate [codegen id : 2]

```

```
Input [2]: [hour, count]
Keys [1]: [hour]
Functions [1]: [finalmerge_count(merge count) AS count(1)]
Aggregate Attributes [1]: [count(1)]
Results [2]: [hour, count(1) AS count]
```

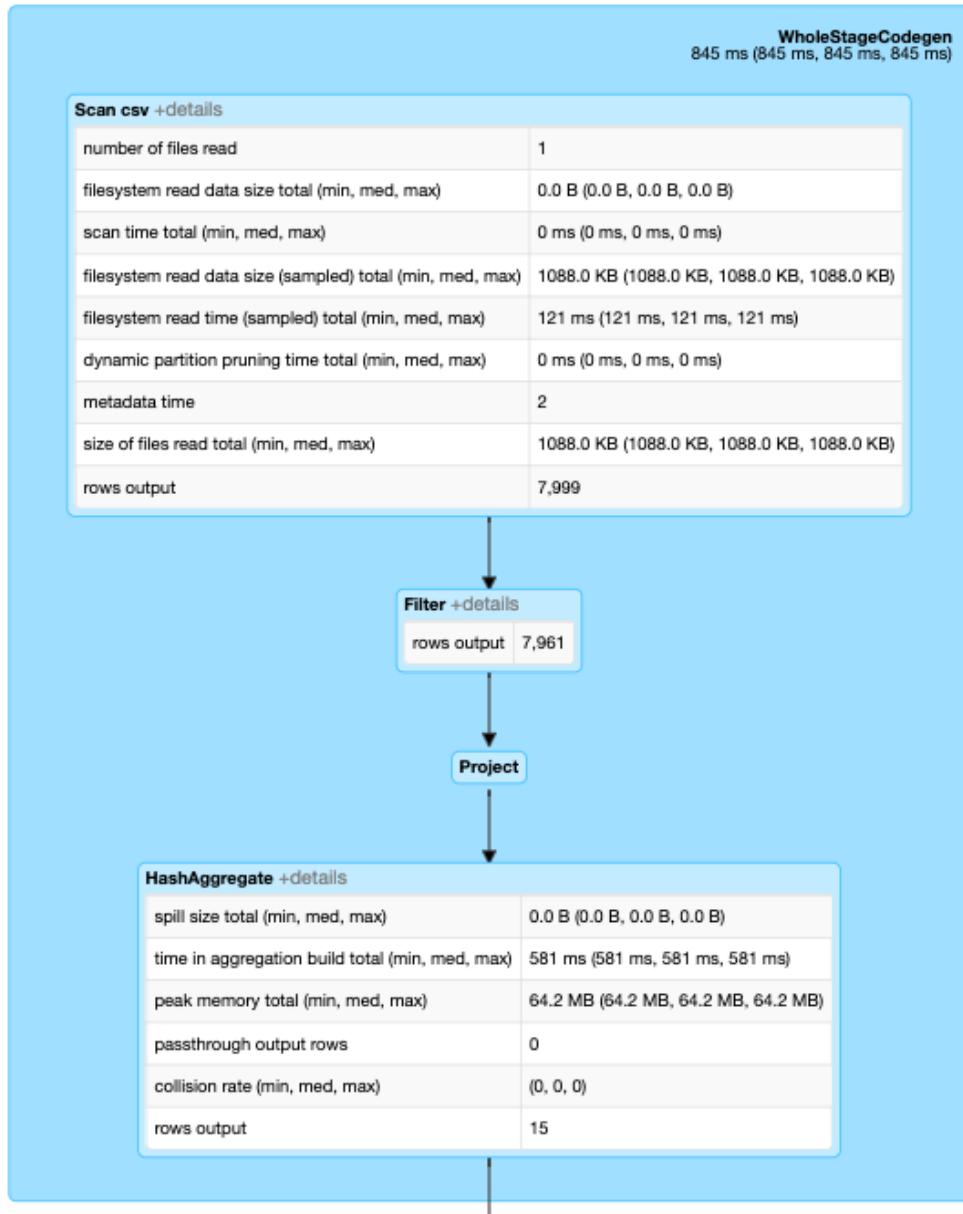


Clicking on the SQL tab link for this query display the DAG of the job.

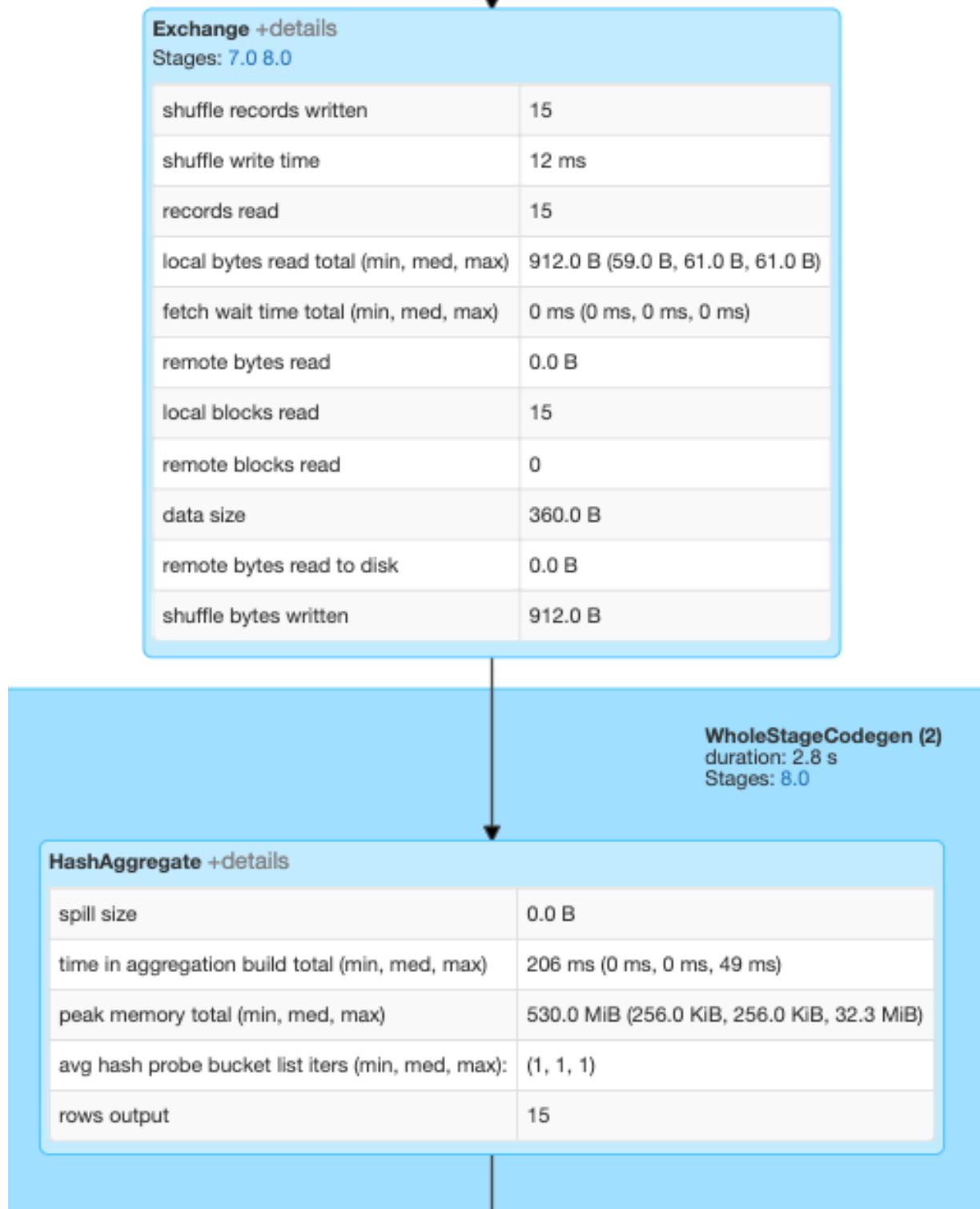


Selecting the **Expand details** checkbox shows detailed information for each stage. The first block **WholeStageCodegen** compiles multiple operators (scan csv, filter, project, and HashAggregate) together into a single Java function to improve performance. Metrics such as number of rows and spill size are shown in the following screen.

Expand all the details in the query plan visualization

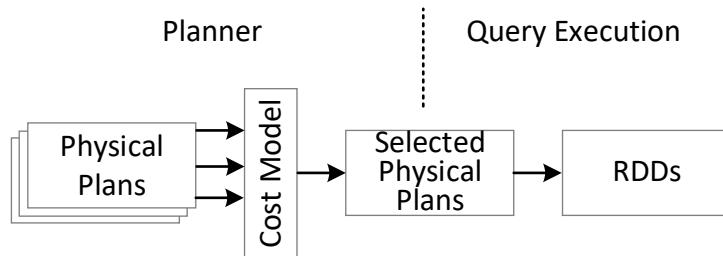


The second block entitled Exchange shows the metrics on the shuffle exchange, including the number of written shuffle records and the data size total.

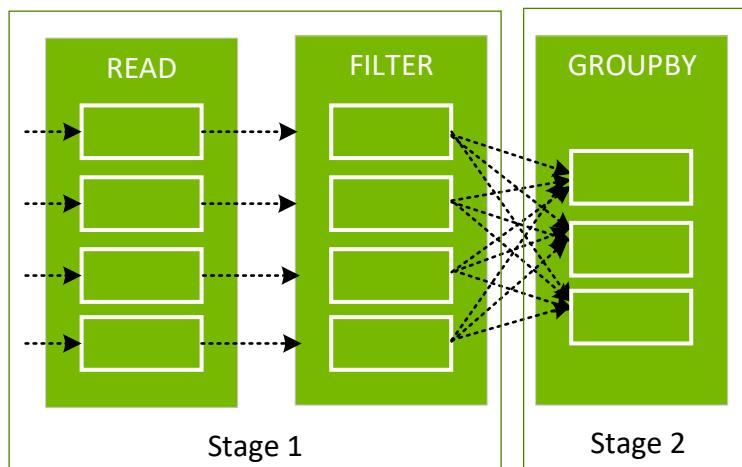


Executing the Tasks on a Cluster

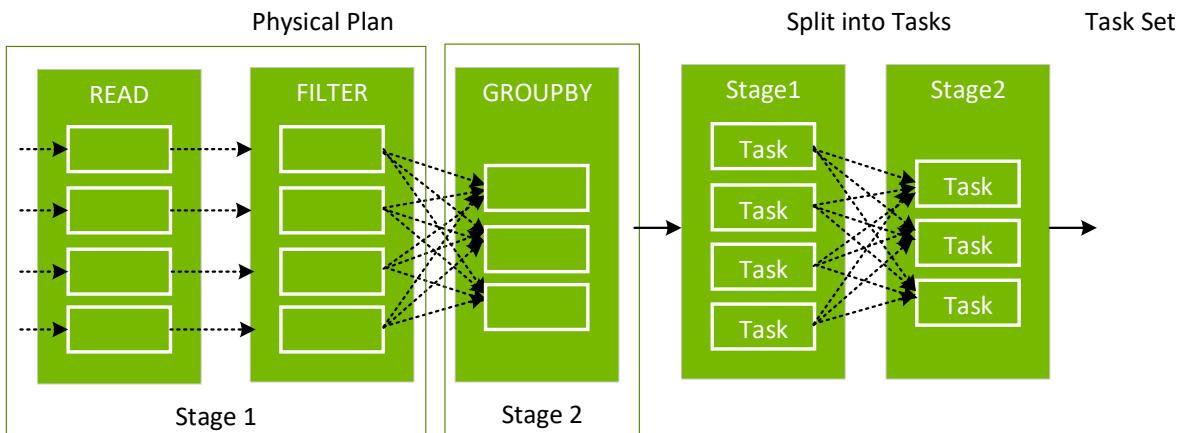
In the third step, the tasks are scheduled and executed on the cluster.



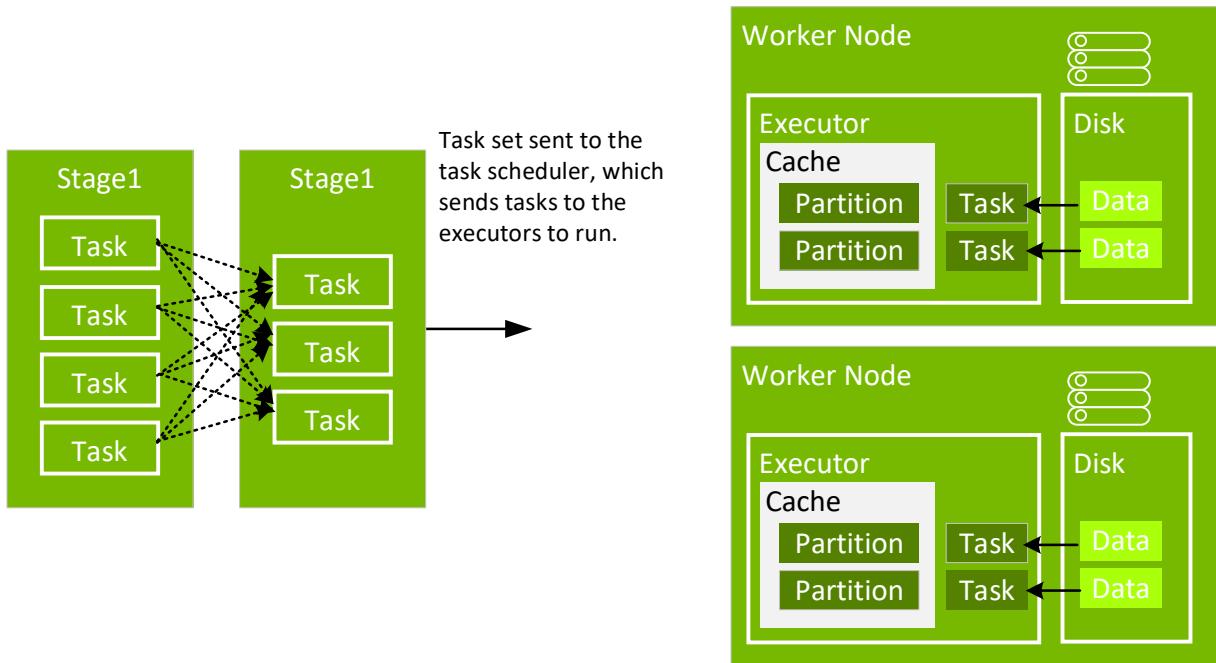
The scheduler splits the graph into stages, based on the transformations. The narrow transformations (transformations without data movement) will be grouped (pipelined) together into a single stage. The physical plan for this example has two stages, with everything before the exchange in the first stage. Spark performs further optimizations at runtime, including **Whole-Stage Java Code Generation**. This optimizes CPU usage by generating a single optimized Java function in bytecode for the set of operators in a SQL query (when possible), instead of generating iterator code for each operator.



Each stage is composed of tasks, based on partitions of the DataFrame, which performs the same computation in parallel.



Next the scheduler submits the stage task set to the task scheduler, which sends tasks to the executors to run.



When the job completes, the action value is returned to the driver, or written to disk, depending on the action.

Clicking the **web UI Jobs** tab gives you details on the progress of the job, including stages and tasks. In the following example, the job consists of two stages, with two tasks in the stage before the shuffle and 200 in the stage after the shuffle. The number of tasks correspond to the partitions. After reading the file in the first stage, there are two partitions.

After a shuffle, the default number of partitions is 200. (You can configure the number of partitions to use when shuffling data with the `spark.sql.shuffle.partitions` property).

Details for Job 1

Status: SUCCEEDED
Associated SQL Query: 23
Job Group: 6985766521759103213_8593600963064183100_eb7954aa2d8345fa8cdabb8e584d2ac3
Completed Stages: 2

► Event Timeline
▼ DAG Visualization

▼ Completed Stages (2)

Stage Id	Pool Name	Description	Submitted	Duration	Tasks: Succeeded/Total	Input	Output	Shuffle Read
2	6985766521759103213	val df3 = df2.groupBy("hour").count df3.orderB... show at command-2718925348255775:3+details	2020/03/18 21:22:56	3 s	200/200			912.0 B
1	6985766521759103213	val df3 = df2.groupBy("hour").count df3.orderB... show at command-2718925348255775:3+details	2020/03/18 21:22:55	1 s	1/1			

Summary

In this chapter, we introduced you to Spark, demonstrated how it executes your code on a cluster, and showed you how to monitor this using the Spark Web UI. Knowing how Spark runs your applications is important when debugging, analyzing, and tuning the performance of your applications.

Chapter 2: Spark SQL and DataFrame Programming

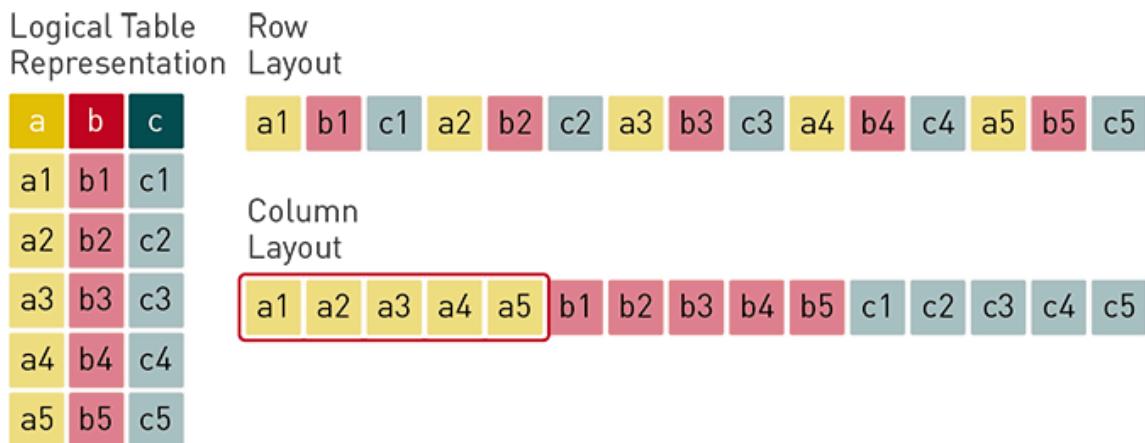
In Chapter 1, we explored how Spark DataFrames execute on a cluster. In this chapter, we'll provide you with an overview of DataFrames and Spark SQL programming, starting with the advantages.

DataFrames and Spark SQL Advantages

The Spark SQL and the DataFrame APIs provide ease of use, space efficiency, and performance gains with Spark SQL's optimized execution engine.

Optimized Memory Usage

Spark SQL caches DataFrames (when you call `dataFrame.cache`) using an in-memory columnar format which is optimized to: scan only required columns, automatically tune compression, minimize memory usage and minimize JVM Garbage Collection.



Spark SQL Vectorized Parquet and ORC readers decompress and decode in column batches, which is roughly nine times faster for reading.

Query Optimization

Spark SQL's Catalyst Optimizer handles logical optimization and physical planning, supporting both rule-based and cost-based optimization. When possible, Spark SQL Whole-Stage Java Code Generation optimizes CPU usage by generating a single optimized function in bytecode for the set of operators in an SQL query.

Exploring the Taxi Dataset with Spark SQL

Data preparation and exploration takes 60 to 80 percent of the analytical pipeline in a typical machine learning (ML) or deep learning (DL) project. In order to build an ML model, you have to clean, extract, explore, and test your dataset in order to find the features of interest that most contribute to the model's accurate predictions. For illustrative purposes, we'll use Spark SQL to explore the Taxi dataset to analyze which features might help predict taxi fare amounts.

Load the Data from a File into a DataFrame and Cache

The following code shows how we loaded the data from a CSV file into a Spark DataFrame, specifying the datasource and schema to load into a DataFrame, as discussed in Chapter 1. After we register the DataFrame as an SQL temporary view, we can use SQL functions on the SparkSession to run SQL queries, which will return the results as a DataFrame. We cache the DataFrame so that Spark does not have to reload it for each query. Also, Spark can cache DataFrames or Tables in columnar format in memory, which can improve memory usage and performance.

Load Data → **DataFrame**

```
// load the data as in Chapter 1
val file = "/data/taxi_small.csv"

val df = spark.read.option("inferSchema", "false")
  .option("header", true).schema(schema).csv(file)

// cache DataFrame in columnar format in memory
df.cache

// create Table view of DataFrame for Spark SQL
df.createOrReplaceTempView("taxi")

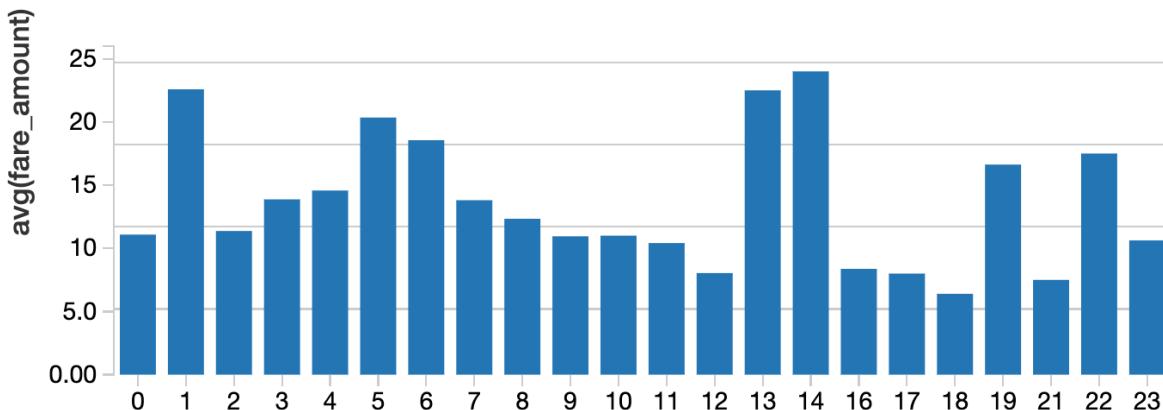
// cache taxi table in columnar format in memory
spark.catalog.cacheTable("taxi")
```

Using Spark SQL

Now we can use Spark SQL to explore what might affect the taxi fare amount, with questions like: What is the average fare amount by hour of the day?

```
%sql
select hour, avg(fare_amount)
from taxi
group by hour order by hour
```

With a notebook like Zeppelin or Jupyter, we can display the SQL results in graph formats.



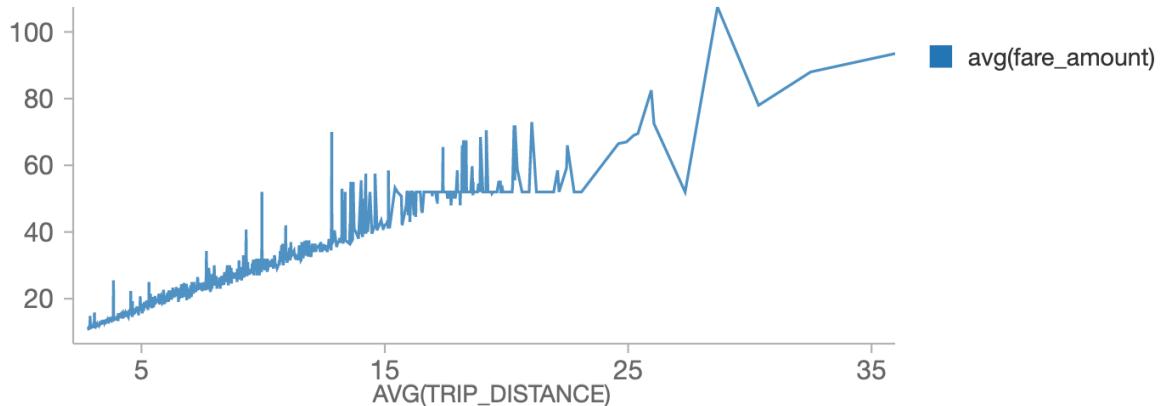
Following is the same query with the DataFrame API:

```
df.groupBy("hour").avg("fare_amount")
.orderBy("hour").show(5)

result:
+-----+
|hour|  avg(fare_amount) |
+-----+
| 0.0|11.08333333333334|
| 1.0|22.581632653061224|
| 2.0|11.370820668693009|
| 3.0|13.873989218328841|
| 4.0| 14.57204433497537|
+-----+
```

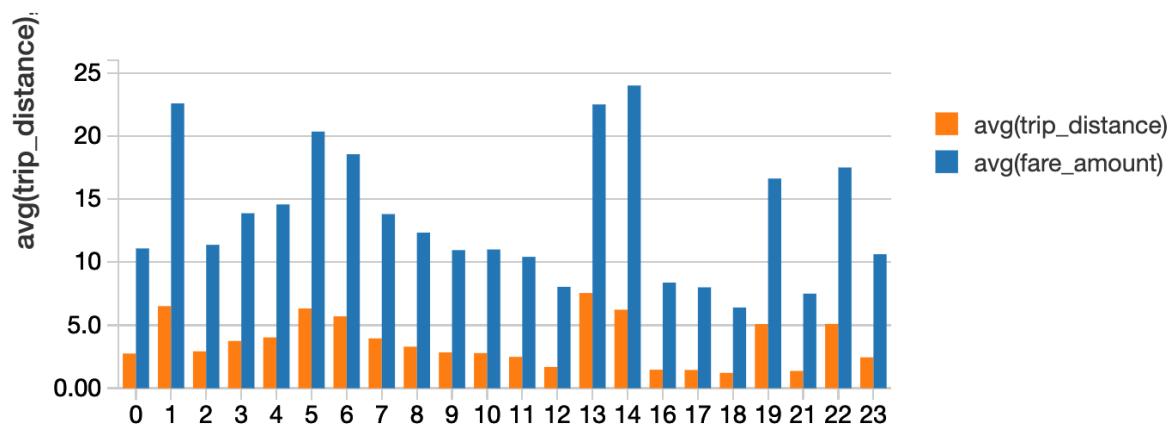
What is the average fare amount compared to the average trip distance?

```
%sql
select trip_distance, avg(trip_distance), avg(fare_amount)
from taxi
group by trip_distance order by avg(trip_distance) desc
```



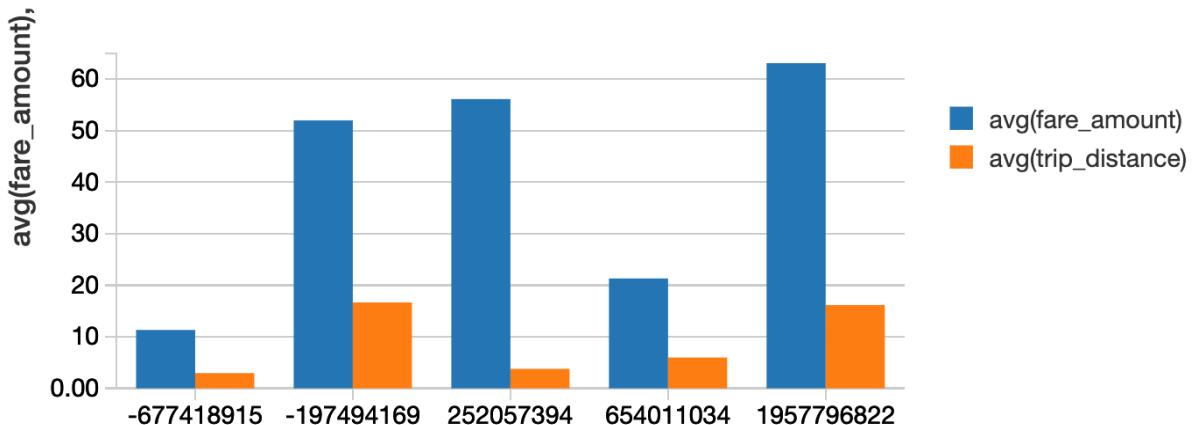
What is the average fare amount and average trip distance by hour of the day?

```
%sql
select hour, avg(fare_amount), avg(trip_distance)
from taxi
group by hour order by hour
```



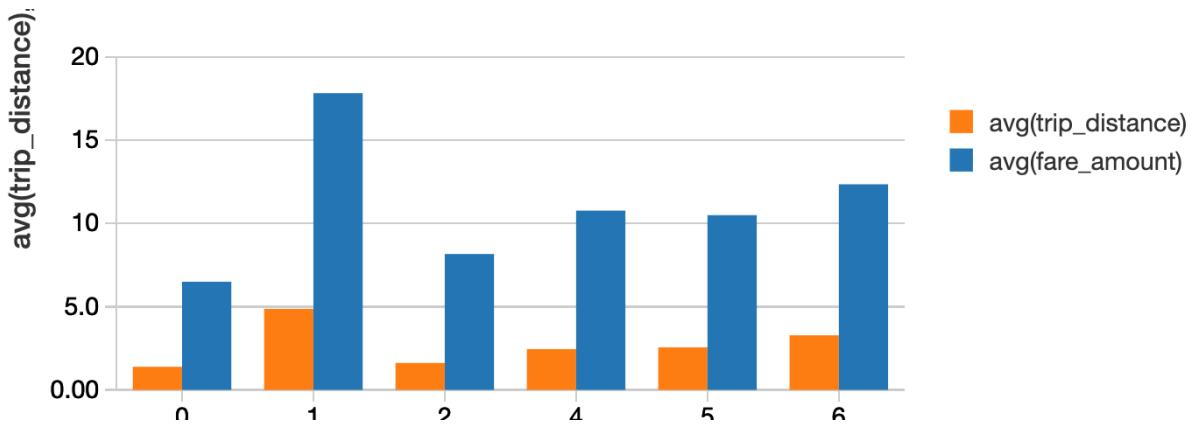
What is the average fare amount and average trip distance by rate code?

```
%sql
select rate_code, avg(fare_amount), avg(trip_distance)
from taxi
group by rate_code order by rate_code
```



What is the average fare amount and average trip distance by day of the week?

```
%sql
select day_of_week, avg(fare_amount), avg(trip_distance)
from taxi
group by day_of_week order by day_of_week
```



Using Spark Web UI to Monitor Spark SQL

SQL Tab

You can use the Spark SQL tab to view Query execution information, such as the query plan details and SQL metrics. Clicking on the query link displays the DAG of the job.



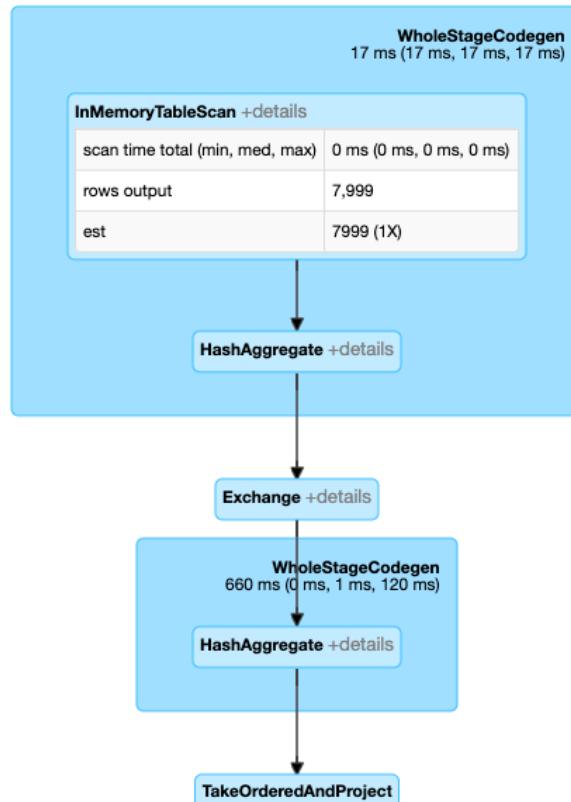
SQL

Completed Queries: 29

Completed Queries (29)

ID	Description	Submitted	Duration	Job IDs
28	tdf.groupBy("hour").avg("fare_amount").orderBy(... +details	2020/03/27 20:18:15	3 s	[9]

Clicking on the +details in the DAG displays details for that stage



Clicking the Details link on the bottom displays the logical plans and the physical plan in text format.

In the query plan details, you can see:

- ▶ The amount of time for each stage.
- ▶ If partition filters, projection, and filter pushdown are occurring.
- ▶ Shuffles between stages (Exchange) and the amount of data shuffled. If joins or aggregations are shuffling a lot of data, consider bucketing.
- ▶ You can set the number of partitions to use when shuffling with the `spark.sql.shuffle.partitions` option.
- ▶ The join algorithm being used. `Broadcast join` should be used when one table is small and `sort-merge join` should be used for large tables. You can use `broadcast` hint to guide Spark to broadcast a table in a join. For faster joins with large tables using the `sort-merge join` algorithm, you can use bucketing to pre-sort and group tables. This will avoid shuffling in the sort merge.

Use the Spark SQL `ANALYZE TABLE tablename COMPUTE STATISTICS` to take advantage of cost-based optimization in the Catalyst Planner.

Jobs Tab

The Jobs tab summary page shows high-level job information, such as the status, duration, and progress of all jobs and the overall event timeline. Here are some metrics to check:

- ▶ **Duration:** Check the amount of time for the job.
- ▶ **Stages succeeded/total tasks, succeeded/total:** Check if there was stage/task failure.

Stages Tab

The Stage tab displays summary metrics for all tasks. You can use the metrics to identify problems with an executor or task distribution. Here are some things to look for:

- ▶ **Duration:** Are there tasks that are taking longer? If your task process time is not balanced, resources could be wasted.
- ▶ **Status:** Are there failed tasks?
- ▶ **Read Size, Write Size:** Is there skew in data size?
- ▶ If your partitions/tasks are not balanced, then consider repartitioning.

Storage Tab

The Storage tab displays DataFrames that are cached or persisted to disk with size in memory and size on disk information. You can use the storage tab to see if cached DataFrames are fitting into memory. If a DataFrame will be reused, and if it fits into memory, caching it will make execution faster.

Executors Tab

The Executors tab displays summary memory, disk, and task usage information by the executors that were created for the application. You can use this tab to confirm that your application has the amount of resources needed, using the following:

- ▶ **Shuffle Read Write Columns:** Shows size of data transferred between stages.
- ▶ **Storage Memory Column:** Features the current used/available memory.
- ▶ **Task Time Column:** Displays task time/garbage collection time.

Partitioning and Bucketing

File partitioning and Bucketing are common optimization techniques in Spark SQL. They can be helpful for reducing data skew and data shuffling by pre-aggregating data in files or directories. DataFrames can be sorted, partitioned, and/or bucketed when saved as persistent tables. Partitioning optimizes reads by storing files in a hierarchy of directories based on the given columns. For example, when we partition a DataFrame by year:

```
df.write.format("parquet")
    .partitionBy("year")
    .option("path", "/data ")
    .saveAsTable("taxi")
```

The directory would have the following structure:

```
path
└── to
    └── table
        ├── year = 2019
        │   ├── part01.parquet
        │   ├── part02.parquet
        ├── year = 2018
        │   ├── part01.parquet
        ...
        :
```

After partitioning the data, when queries are made with filter operators on the partition column, the Spark SQL catalyst optimizer pushes down the partition filter to the datasource. The scan reads only the directories that match the partition filters, reducing disk I/O and data loaded into memory. For example, the following query reads only the files in the year = '2019' directory.

```
df.filter("year = '2019'")
    .groupBy("year").avg("fareamount")
```

When visualizing the physical plan for this query, you will see `Scan PrunedInMemoryFileIndex[/data/year=2019], PartitionFilters: [(year = 2019)]`.

Similar to partitioning, bucketing splits data by a value. However, bucketing distributes data across a fixed number of buckets by a hash on the bucket value, whereas partitioning creates a directory for each partition column value. Tables can be bucketed on more than one value and bucketing can be used with or without partitioning. If we add bucketing to the previous example, the directory structure is the same as before, with data files in the year directories grouped across four buckets by hour.

```
df.write.format("parquet")
    .partitionBy("year")
    .bucketBy(4, "hour")
    .option("path", "/data ")
    .saveAsTable("taxi")
```

After bucketing the data, aggregations and joins (wide transformations) on the bucketed value do not have to shuffle data between partitions, reducing network and disk I/O. Also, bucket filter pruning will be pushed to the datasource reducing disk I/O and data loaded into memory. The following query pushes down the partition filter on year to the datasource and avoids the shuffle to aggregate on hour.

```
df.filter("year = '2019'")
    .groupBy("hour")
    .avg("hour")
```

Partitioning should only be used with columns used frequently in queries for filtering and that have a limited number of column values with enough corresponding data to distribute the files in the directories. Small files are less efficient with excessive parallelism and too few large files can hurt parallelism. Bucketing works well when the number of unique bucketing column values is large and the bucketing column is used often in queries.

Summary

In this chapter, we explored how to use tabular data with Spark SQL. These code examples can be reused as the foundation for processing data with Spark SQL. In another chapter, we use the same data with DataFrames for predicting taxi fares.

Chapter 3: GPU-Accelerated Apache Spark 3.x

Spark 3.x and GPUs

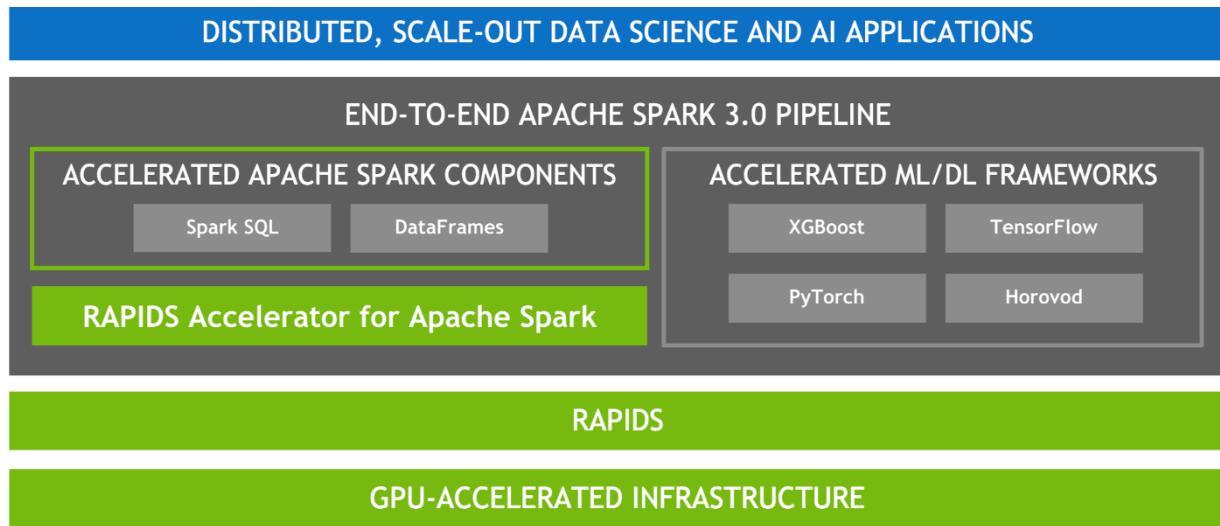
Given the parallel nature of many data processing tasks, it's only natural that the massively parallel architecture of a GPU should be able to parallelize and accelerate Spark data processing queries, in the same way that a GPU accelerates deep learning (DL) in artificial intelligence (AI). Therefore, NVIDIA® has worked with the Spark community to implement GPU acceleration as part of Spark 3.x.

While Spark distributes computation across nodes in the form of partitions, within a partition, computation has historically been performed on CPU cores. However, the benefits of GPU acceleration in Spark are many. For one, fewer servers are required, reducing infrastructure cost. And, because queries are completed faster, you expect a reduction in time to results. Also, since GPU acceleration is transparent, applications built to run on Spark require no changes in order to reap the benefits of GPU acceleration.

Accelerated ETL and AI in Spark

As machine learning (ML) and DL are increasingly applied to larger datasets, Spark has become a commonly used vehicle for the data pre-processing and feature engineering needed to prepare raw input data for the learning phase. The Spark community has been focused on bringing both phases of this end-to-end pipeline together, so that data scientists can work with a single Spark cluster and avoid the penalty of moving data between phases via an external data lake. [Horovod](#) (by Uber) and [TensorFlowOnSpark](#) (by Yahoo) are examples of this approach.

Spark 3.x represents a key milestone, as Spark can now schedule GPU-accelerated ML and DL applications on Spark clusters with GPUs. The complete Spark 3 software stack that includes the RAPIDS Accelerator for Apache Spark is shown in the following figure.



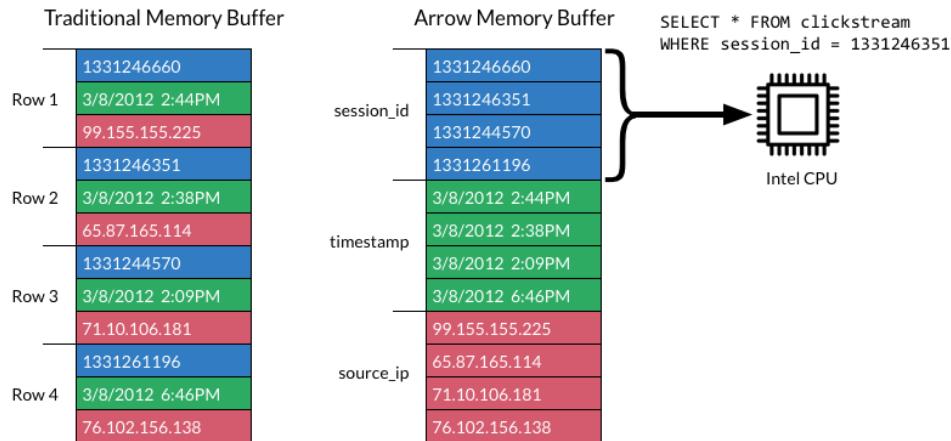
New GPU-Accelerated Libraries on NVIDIA CUDA

As discussed previously, [NVIDIA® CUDA®](#) is a programming model and a set of APIs for accelerating operations on the NVIDIA GPU architecture. Layered on top of CUDA, RAPIDS is a suite of open-source software libraries and APIs that provide GPU parallelism and high-bandwidth memory speed through DataFrame and graph operations.

RAPIDS GPU-Accelerated Spark DataFrames

RAPIDS offers a powerful GPU DataFrame based on [Apache Arrow](#) data structures. Arrow specifies a standardized, language-independent, columnar memory format, optimized for data locality, to accelerate analytical processing performance on modern CPUs or GPUs. With the GPU DataFrame, batches of column values from multiple records take advantage of modern GPU designs and accelerate reading, queries, and writing.

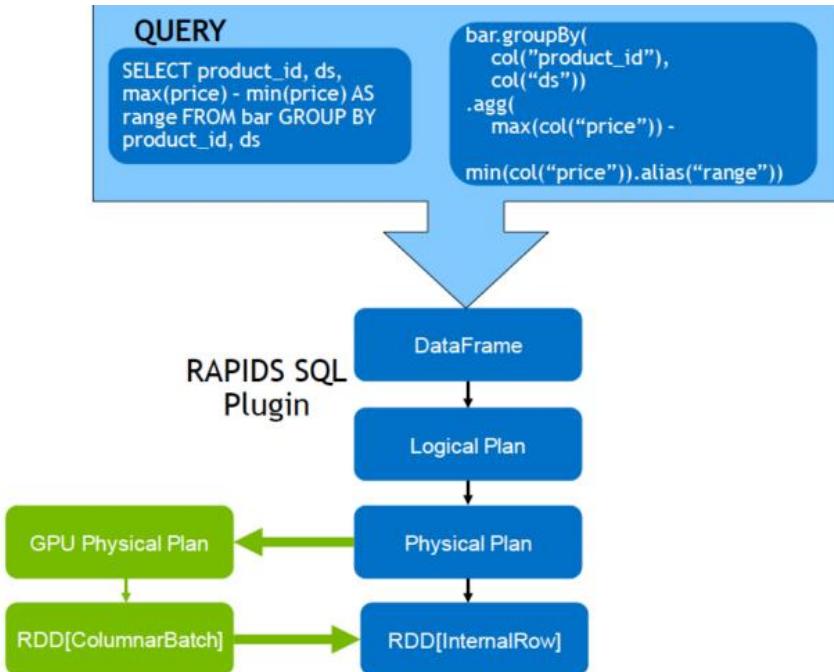
	session_id	timestamp	source_ip
Row 1	1331246660	3/8/2012 2:44PM	99.155.155.225
Row 2	1331246351	3/8/2012 2:38PM	65.87.165.114
Row 3	1331244570	3/8/2012 2:09PM	71.10.106.181
Row 4	1331261196	3/8/2012 6:46PM	76.102.156.138



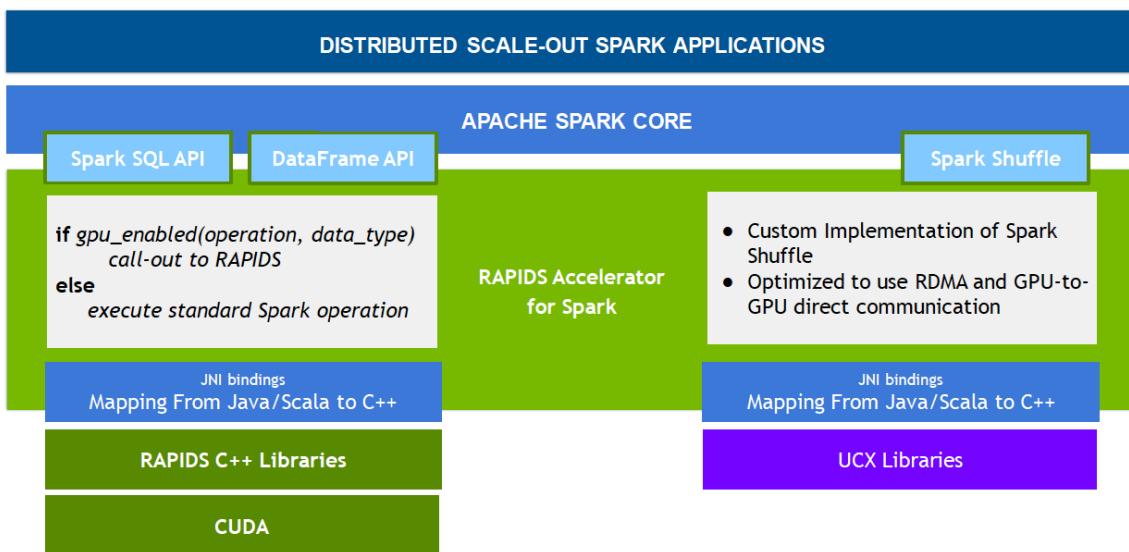
Spark GPU-Accelerated DataFrame and SQL

For Apache Spark 3.0, new RAPIDS APIs are used by Spark SQL and DataFrames for GPU-accelerated memory-efficient columnar data processing and query plans. With the RAPIDS accelerator, the Catalyst query optimizer plugin interface has been extended to identify operators within a query plan that can be accelerated with the RAPIDS API, mostly a one-to-one mapping, and to schedule those operators on GPUs within the Spark cluster when executing the query plan.

With a physical plan for CPUs, the DataFrame data is transformed into RDD row format and usually processed one row at a time. Spark supports columnar batch, but in Spark 2.x only the Vectorized Parquet and ORC readers use it. The RAPIDS plugin extends columnar batch processing on GPUs to most Spark operations. Processing columnar data is much more GPU friendly than row-by-row processing.



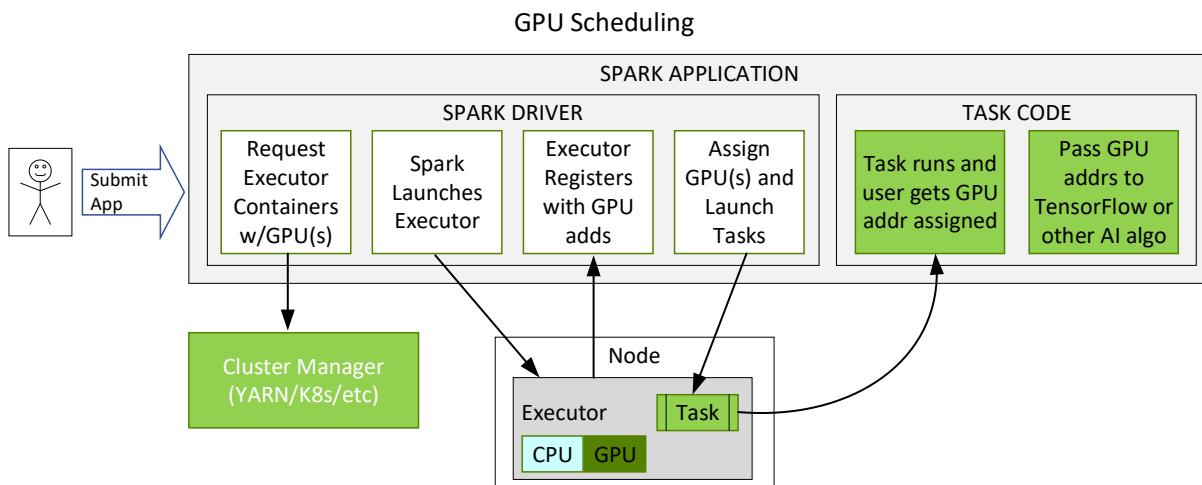
A new Spark shuffle implementation built upon OpenUCX communication libraries leverage NVLink, RDMA and InfiniBand (if available) to dramatically reduce data transfer among Spark processes by: keeping as much data on the GPU as possible, finding the fastest path to move data between nodes, using the best of available hardware resources, including bypassing the CPU to do GPU to GPU memory intra and inter node transfers. RDMA allows GPUs to transfer data directly across nodes at up to PCIe speeds, operating as if on one massive server. NVLink allows GPUs to initiate peer to peer communication at up to 300GB/s.



GPU-Aware Scheduling in Spark

Spark 3.x adds integration with the YARN, Kubernetes, and Standalone cluster managers to request GPUs and plugin points, which can be extended to run operations on GPUs. For Kubernetes, Spark 3.x offers GPU isolation at the executor pod level. This makes GPUs easier to request and use for Spark application developers, allows for closer integration with DL and AI frameworks like Horovod and TensorFlow on Spark, and allows for better utilization of GPUs.

An example of a flow for GPU scheduling is shown in the diagram below. The user submits an application with a GPU resource configuration discovery script. Spark starts the driver, which uses the configuration to pass on to the cluster manager, to request a container with a specified amount of resources and GPUs. The cluster manager returns the container. Spark launches the container. When the executor starts, it will run the discovery script. Spark sends that information back to the driver and the driver can then use that information to schedule tasks to GPUs.



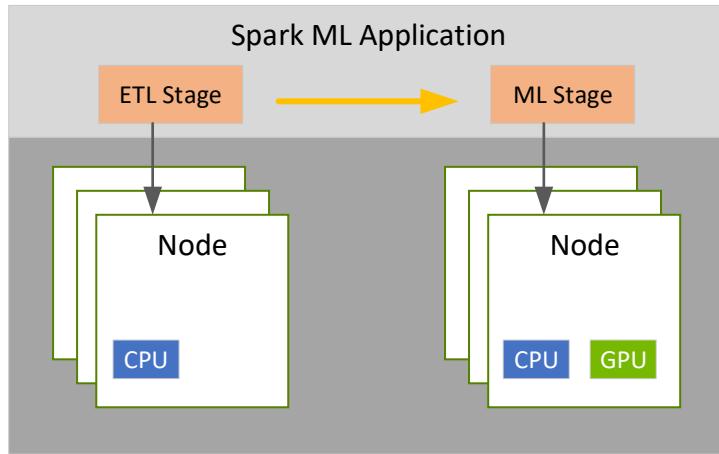
The Spark Web UI has been modified with a new checkbox to see which resources have been allocated. In this instance, two GPUs have been allocated.

The screenshot shows the Spark Web UI Executors page. A green arrow points to the 'Resources' checkbox in the 'Show Additional Metrics' section, which is checked. Another green arrow points down to the table showing executor details, where 'gpu: [0, 1]' is listed under the 'Resources' column for the 'driver' executor.

Executor ID	Address	Status	RDD Blocks	Storage Memory	Disk Used	Cores	Active Tasks	Failed Tasks	Complete Tasks	Total Tasks	Task Time (GC Time)	Input	Shuffle Read	Shuffle Write	Blacklisted
Active(2)	0	0.0 B / 8.7 GiB	0.0 B	2	0	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	0	
Dead(0)	0	0.0 B / 0.0 B	0.0 B	0	0	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	0	
Total(2)	0	0.0 B / 8.7 GiB	0.0 B	2	0	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	0	

Executor	ID	Address	Status	RDD Blocks	Storage Memory	Disk Used	Cores	Resources	Active Tasks	Failed Tasks	Complete Tasks	Total Tasks	Task Time (GC Time)	Input	Shuffle Read	Shuffle Write	Thread Dump Logs
driver	10.28.9.112:42305	Active	0	0.0 B / 8.4 GiB	0.0 B	0	0	gpu: [0, 1]	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	Thread Dump
1	tong-x299-37047	Active	0	0.0 B / 366.3 MiB	0.0 B	2	gpu: [0, 1]	0	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	stdout Thread Dump

Spark 3.x stage level resource scheduling allows you to choose one container size for one stage and another size for another stage. For example, one for ETL and another for ML.



XGBoost, RAPIDS, and Spark

XGBoost is a scalable, distributed gradient-boosted decision tree (GBDT) ML library. XGBoost provides parallel tree boosting and is the leading ML library for regression, classification, and ranking problems. The RAPIDS team works closely with the Distributed Machine Learning Common (DMLC) XGBoost organization, and XGBoost now includes seamless, drop-in GPU acceleration, significantly speeding up model training and improving accuracy for better predictions.

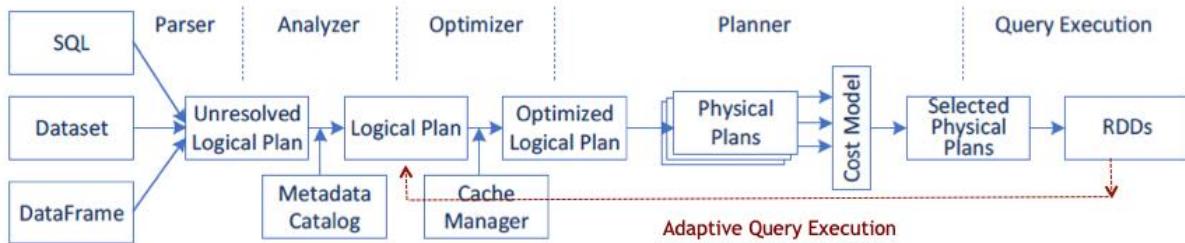
RAPIDS, XGBOOST, and SPARK has three features that help with speed-up and cost:

- ▶ **GPU-accelerated DataFrame:** Reads any number/size of supported input file formats directly into GPU memory and divides up evenly among the different training nodes.
- ▶ **GPU-accelerated training:** XGBoost training time has been improved with a dynamic in-memory representation of the training data that optimally stores features based on the sparsity of a dataset. This replaces a fixed in-memory representation based on the largest number of features amongst different training instances.
- ▶ **Efficient GPU memory utilization:** XGBoost requires that data fit into memory which creates a restriction on data size using either a single GPU or distributed multi-GPU multi-node training. The latest release has improved GPU memory utilization by 5X. Now users can train with data that is five times the size as compared to the first version. This improves total cost of training without impacting performance.

Later in this eBook, we explore and discuss an example using the upgraded XGBoost library to load/transform data and conduct distributed training using GPUs.

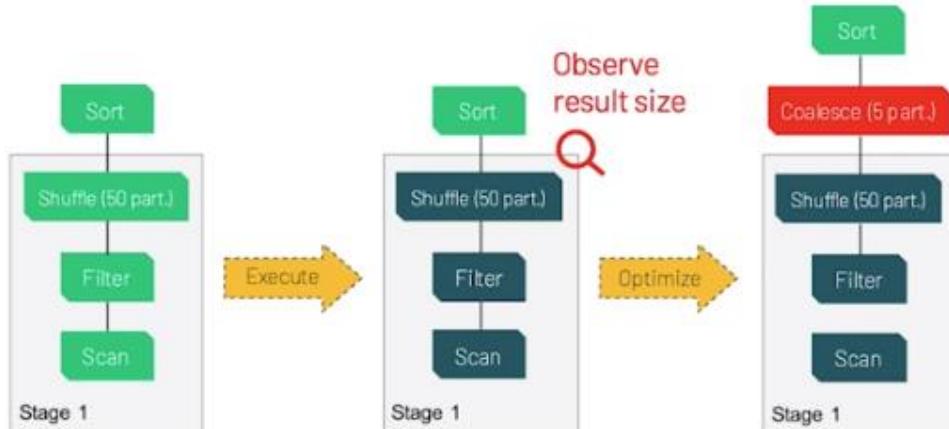
Other Spark 3.x Features

- **Adaptive Query execution:** Spark 2.2 added cost-based optimization to the existing rule based SQL Optimizer. Spark 3.0 now has runtime adaptive query execution(AQE). With AQE, runtime statistics retrieved from completed stages of the query plan are used to re-optimize the execution plan of the remaining query stages. Databricks benchmarks yielded speed-ups ranging from 1.1x to 8x when using AQE.

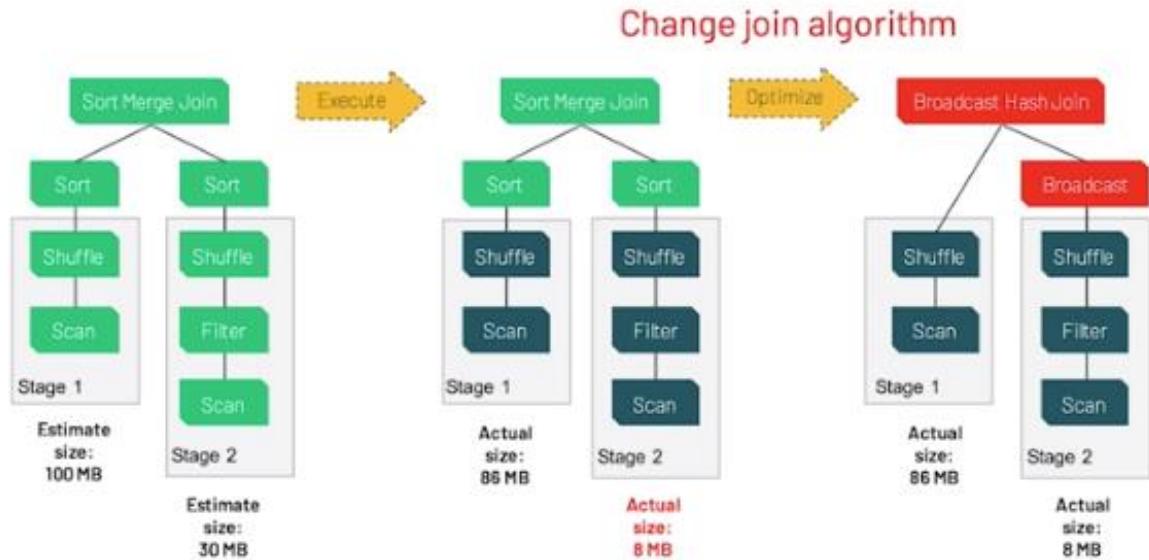


Spark 3.0 AQE optimization features include:

- Dynamically coalesce shuffle partitions: AQE can combine adjacent small partitions into bigger partitions in the shuffle stage by looking at the shuffle file statistics, reducing the number of tasks for query aggregations.

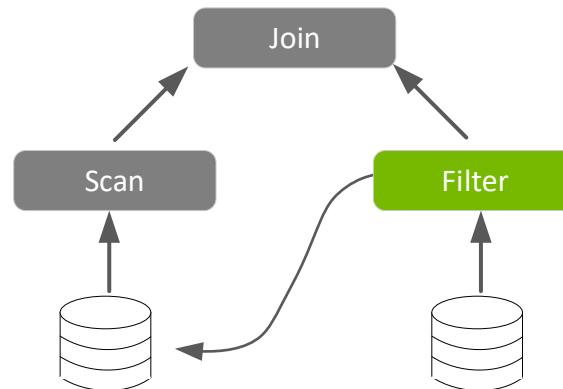


- Dynamically switch join strategies: AQE can optimize the join strategy at runtime based on the join relation size. For example, converting a sort merge join to a broadcast hash join which performs better if one side of the join is small enough to fit in memory.



- Dynamically optimize skew joins: AQE can detect data skew in sort-merge join partition sizes using runtime statistics and split skew partitions into smaller sub-partitions.
- ▶ **Dynamic Partition Pruning:** Partition pruning is a performance optimization that limits the number of files and partitions that Spark reads when querying. After partitioning the data, queries that match certain partition filter criteria improve performance by allowing Spark to only read a subset of the directories and files. Spark 3.0 dynamic partition pruning allows the Spark engine to dynamically infer, at runtime, the specific partitions within a table that need to be read and processed for a specific query, by identifying the partition column values that result from filtering another table in a join. For example, the following query involves two tables: the `flight_sales` table that contains all of the total sales for all flights, partitioned by originating airport, and the `flight_airports` table that contains a mapping of airports for each region. Here we are querying for sales in the North-East America region.

```
select fs.airport, fs.total_sales
from flight_sales fs, flight_airports fa
where fs.airport = fa.airport and fa.region = 'NEUSA'
```



With dynamic partition pruning, this query will scan and process only the partitions for the airports returned by the where filter on the region. Reducing the amount of data read and processed results in a significant time savings.

- ▶ Join strategy hints instruct the optimizer to use the hinted plan for join strategies. MERGE, SHUFFLE_HASH and SHUFFLE_REPLICATE_NL hints were added to the existing BROADCAST hint.
- ▶ DataSource API Improvements:
 - Pluggable catalog integration.
 - Improved predicate push down for faster queries via reduced data loading.

Summary

In this chapter, we covered the main improvements in Spark 3.x that are proving instrumental in accelerating time to insights, especially when executed on NVIDIA GPUs. Details on new Spark 3.0 features can be found in the [Spark 3.0 release notes](#).

Chapter 4: Getting Started with GPU-Accelerated Apache Spark 3.x

In Chapter 3, we discussed the features of GPU-Acceleration in Spark 3.x. In this chapter, we go over the basics of getting started using the new RAPIDS Accelerator for Apache Spark 3.x that leverages GPUs to accelerate processing via the [RAPIDS libraries](#) (For details refer to the [Getting Started with the RAPIDS Accelerator for Apache Spark](#)).

The RAPIDS Accelerator for Apache Spark has the following features and limitations:

- ▶ Allows running Spark SQL on a GPU with Columnar processing
- ▶ Requires no API changes from the user
- ▶ Handles transitioning from Row to Columnar and back
- ▶ Uses Rapids cuDF library
- ▶ Runs supported SQL operations on the GPU, If an operation is not implemented or not compatible with GPU, it will fall back to using the Spark CPU version.
- ▶ The plugin cannot accelerate operations that manipulate RDDs directly.
- ▶ The accelerator library also provides an implementation of Spark's shuffle that can leverage UCX to optimize GPU data transfers keeping as much data on the GPU as possible and bypassing the CPU to do GPU to GPU transfers.

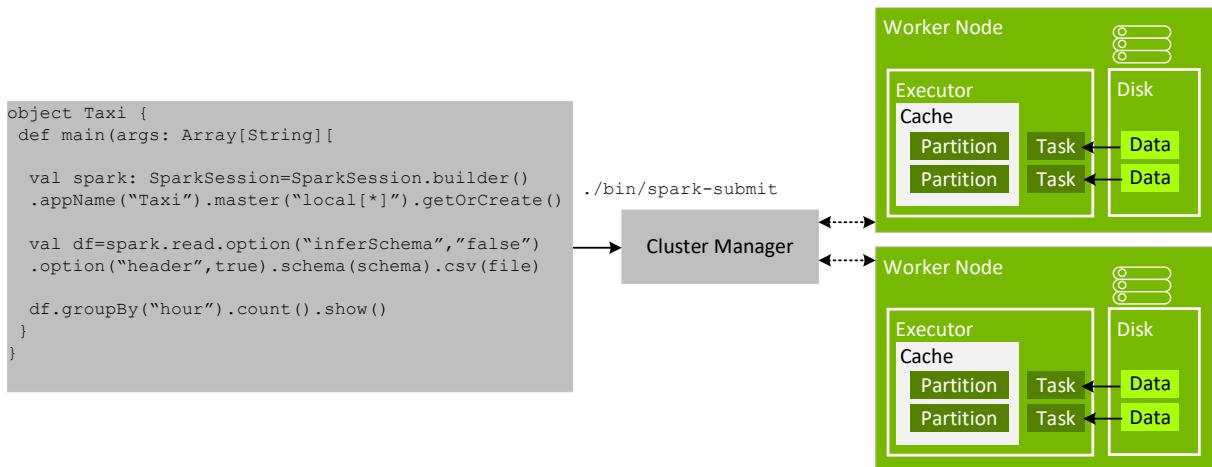
To enable this GPU acceleration, you will need:

- ▶ Apache Spark 3.0+
- ▶ A spark cluster configured with GPUs that comply with the requirements for the version of [RAPIDS Dataframe library cuDF](#).
 - One GPU per executor.
- ▶ Add the following jars:
 - A cudf jar that corresponds to the version of CUDA available on your cluster.
 - RAPIDS Spark accelerator plugin jar.
- ▶ Set the config `spark.plugins` to `com.nvidia.spark.SQLPlugin`

Installation and Configuration

The way you deploy Spark affects the steps you must take to install and setup Spark and the RAPIDS Accelerator for Spark. The primary methods to deploy Spark are:

- ▶ Local mode - the driver program and tasks run in the same Java Virtual Machine. This is useful for development and testing only, it is not meant for running production applications.
- ▶ On a Cluster with a cluster manager:
 - Standalone Deploy Mode: simplest way to deploy Spark on a private cluster
 - Hadoop YARN
 - Kubernetes



Installation

For installation basically you need Spark 3.x, the RAPIDS Accelerator for Spark jars, and a GPU discovery script available on every worker node. With Local you install these locally. With Spark Standalone, you install these on all the nodes you will use. With Yarn you install these on a launcher node and YARN handles shipping them to the nodes as needed. With Kubernetes you either put everything you need in a docker image, or on a drive that is mounted when your Spark application runs. For details on installation refer to the [Getting Started with the RAPIDS Accelerator for Apache Spark](#).

Configuration

The Spark shell and `./bin/spark-submit` support loading configuration properties dynamically, via command line options, such as `--conf`, or by reading configuration options from `conf/spark-defaults.conf`. (Refer to the [Spark Configuration Guide](#) for an overview and details on Spark configurations.)

On startup use: --conf [conf key]=[conf value]. For example:

```
 ${SPARK_HOME}/bin/spark --jars 'rapids-4-spark_2.12-0.1.0.jar,cudf-0.14.jar'
 \
 --conf spark.plugins=com.nvidia.spark.SQLPlugin \
 --conf spark.rapids.sql.incompatibleOps.enabled=true
```

At runtime use: spark.conf.set("[conf key]", [conf value]). For example:

```
 scala> spark.conf.set("spark.rapids.sql.incompatibleOps.enabled", true)
```

GPU Scheduling

You can use --conf key value pairs to request GPUs and assign them to tasks. The exact configuration you use will vary depending on your cluster manager. Here are a few of the configuration key value properties for assigning GPUs:

- ▶ Request your executor to have GPUs:

```
--conf spark.executor.resource.gpu.amount=1
```

- ▶ Specify the number of GPUs per task:

```
--conf spark.task.resource.gpu.amount=1
```

- ▶ Specify a discoveryScript (required on YARN and K8S):

```
--conf spark.executor.resource.gpu.discoveryScript=./getGpusResources.sh
```

Note that spark.task.resource.gpu.amount can be a decimal amount, so if you want multiple tasks to be run on an executor at the same time and assigned to the same GPU you can set this to a decimal value less than 1. You would want this setting to correspond to the spark.executor.cores setting. For instance, if you have spark.executor.cores=2 which would allow 2 tasks to run on each executor and you want those 2 tasks to run on the same GPU then you would set spark.task.resource.gpu.amount=0.5.

Tuning

The following configs are recommended to get started but must be configured based on your cluster and application:

- ▶ Run with one Executor per GPU. Do not try to run with multiple GPUs per executor. Each executor can run with multiple tasks, this depends on the number of cores and number of GPUs on each of your boxes. Run one executor per GPU and you can evenly divide your cores among your executors. For instance, if you have 24 cores and four GPUs per host, you can run with six cores (--conf spark.executor.cores=6). This controls the number of tasks that Spark puts on an executor at once. To control the number of tasks that are concurrently running on the GPU at once you can configure spark.rapids.sql.concurrentGpuTasks. A good starting point is to allow two tasks to run on the GPU concurrently:

```
(--conf spark.rapids.sql.concurrentGpuTasks=2),
```

If you have issues with out-of-memory or slow performance change this to 1. The reason for the difference is that the tasks can still use the CPU while other tasks are running on the GPU. Currently we do not get a performance benefit from running too many tasks on the GPU at once and each of those will be using memory, so we generally limit the number on the GPU at once.

- ▶ Set the size of the input. You will realize a performance improvement when you run bigger batches of data on your GPUs. However, your input size will depend on the type of file you are reading from and the operation you are performing.

- If you are using the Spark datasource api (spark.read...), use:

```
--conf spark.sql.files.maxPartitionBytes=512m
```

- If you are using Spark/Hive api to read data from a Hive Table, use:

```
--conf  
spark.hadoop.mapreduce.input.fileinputformat.split.minsize=536870912  
--conf spark.hadoop.mapred.min.split.size=536870912
```

- ▶ Configure the number of `spark.sql.shuffle.partitions`. Spark defaults to 200, which many times results in very small partitions. You want the data size of each partition to be large to make processing on the GPU efficient, so try to keep the number of partitions to as few as possible. Tune this along with the input size based on your application data.

If you are using the KryoSerializer with Spark

```
(--conf spark.serializer=org.apache.spark.serializer.KryoSerializer)
```

you need to register the `GpuKryoRegistrar` class, e.g.:

```
--conf spark.kryo.registrator=com.nvidia.spark.rapids.GpuKryoRegistrar
```

- ▶ Configure the amount of executor memory like you would for a normal Spark application.

General Recommendations

- ▶ Fewer large input files are better than lots of small files. You may not have control over this but it is worth knowing.
- ▶ Larger input sizes `spark.sql.files.maxPartitionBytes=512m` are generally better as long as things fit into the GPU.
- ▶ The GPU does better with larger data chunks as long as they fit into memory. When using the default `spark.sql.shuffle.partitions=200` it may be beneficial to make this smaller. Base this on the amount of data the task is reading. Start with 512MB / task.

Advanced Configuration

Beyond the configurations, we have other plugin-specific configurations that may help performance as long as certain requirements are met. These configurations control what operations can run on the GPU (see the following Table). Enabling these allows more things to be optimized and run on the GPU, but make sure to understand what they do. For instance, the GPU may not be 100% compatible with the CPU version. For instance, floating point numbers may be slightly different. For more details on configuration refer to the [RAPIDS Accelerator for Spark Configuration](#).

Monitoring Using the Physical Plan

The RAPIDS Accelerator for Spark requires no API changes from the user, and it will replace SQL operations it supports with GPU operations. In order to see what operations were replaced with GPU operations, you can print out the physical plan for a DataFrame by calling the `explain` method, all of the operations prefixed with GPU take place on GPUs.

Now, compare the physical plan for a DataFrame with GPU processing for some of the same queries we looked at in Chapter 1. In the physical plan below, the DAG consists of a `GpuBatchScan`, a `GpuFilter` on `hour`, and a `GpuProject` (selecting columns) on `hour`, `fare_amount`, and `day_of_week`. With CPU processing it consisted of a `FileScan`, `Filter`, and a `Project`.

```
// select and filter are narrow transformations
df.select($"hour", $"fare_amount").filter($"hour" === "0.0").show(2)

result:
+-----+
|hour|fare_amount|
+-----+
| 0.0|      10.5|
| 0.0|      12.5|
+-----+

df.select($"hour", $"fare_amount").filter($"hour" === "0.0").explain

result:
== Physical Plan ==
*(1) GpuColumnarToRow false
+- !GpuProject [hour#10, fare_amount#9]
  +- GpuCoalesceBatches TargetSize(1000000,2147483647)
    +- !GpuFilter (gpuisnotnull(hour#10) AND (hour#10 = 0.0))
      +- GpuBatchScan[fare_amount#9, hour#10] GpuCSVScan Location:
InMemoryFileIndex[s3a://spark-taxi-dataset/raw-small/train], ReadSchema:
struct<fare_amount:double,hour:double>
```

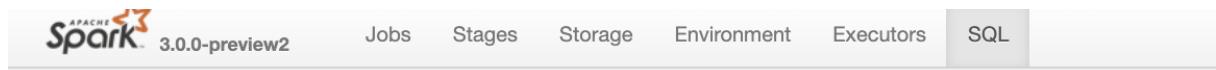
Notice how most of the nodes in the original plan have been replaced with GPU versions. The RAPIDS Accelerator inserts data format conversion nodes, like `GpuColumnarToRow` and `GpuRowToColumnar` to convert between columnar processing for nodes that will execute on the GPU and row processing for nodes that will execute on the CPU. To see why some parts of your query did not run on the GPU set the config `spark.rapids.sql.explain` to true. The output will be logged to the driver's log or to the screen in interactive mode.

Monitoring Using the Spark Web UI

SQL Tab

The easiest way to see what is running on the GPU is to look at the "SQL" tab in the Spark Web UI. In the DAG diagram from the SQL Tab for the query below, we see that the physical plan consists of a GPUBatchScan, Project, GPUHashAggregate, and a GPUHashAggregate. With CPU processing Spark performs a hash aggregation for each partition before shuffling the data in the Exchange for the wide transformation. After the exchange, there is a hash aggregation of the previous sub-aggregations. Note that for GPU processing the Exchange shuffle has been avoided.

```
val df3 = df2.groupBy("month").count  
.orderBy(asc("month")) show(5)
```

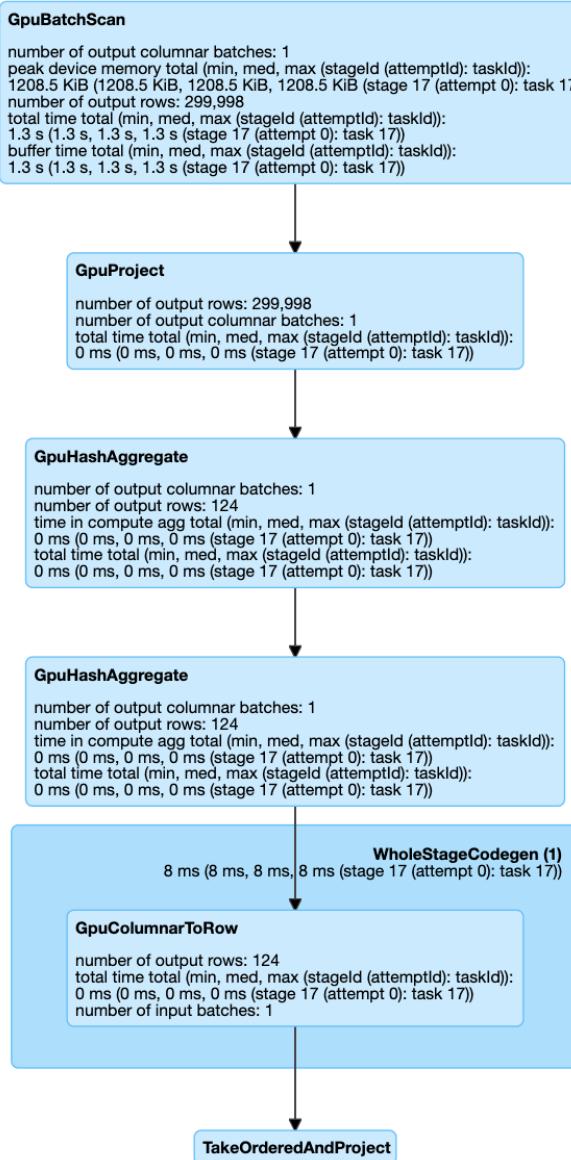


Details for Query 17

Submitted Time: 2020/04/20 19:58:19

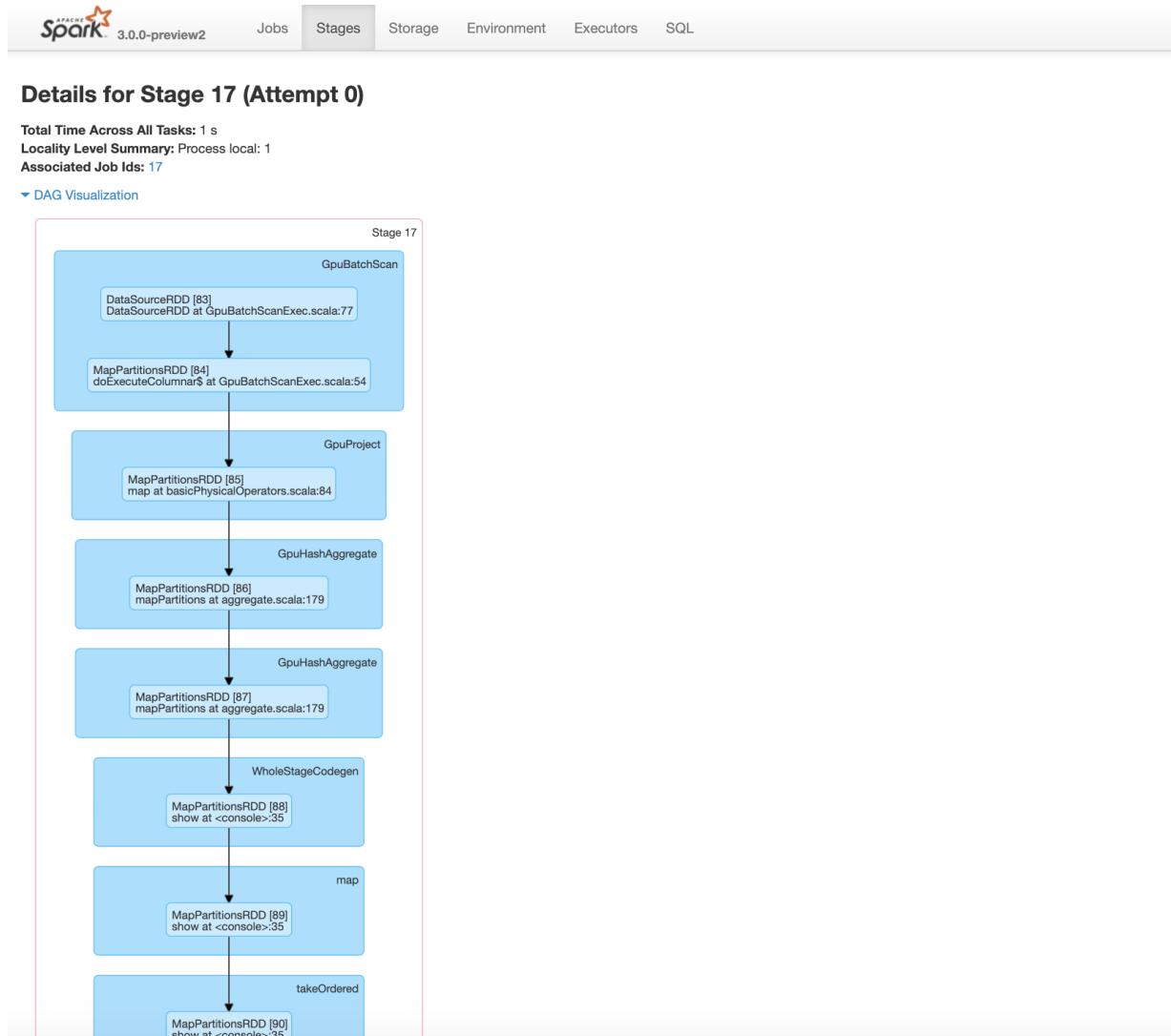
Duration: 2 s

Succeeded Jobs: 17



Stages Tab

You can use the stage details page to view a stage details DAG, where the blue vertices (boxes) represent the RDDs or DataFrames and the edges (arrows between boxes) represent the operation applied to a DataFrame.



Environment Tab

You can use the Environment tab to view and check whether the GPU configuration your properties have been set correctly, for example the `Spark.executor.resource.gpu.amount` and `spark.executor.resource.gpu.discoveryScript` properties. Here you can also view the System Properties classpath entries to check that the plugin jars are in the JVM classpath.

Table 1. Spark Properties

Name	Value
<code>spark.executor.resource.gpu.amount</code>	1
<code>spark.executor.resource.gpu.discoveryScript</code>	/home/ubuntu/getGpusResources.sh

Executors Tab

You can use the Executors tab to see which resources have been allocated for the executors for your application. In this instance, one GPUs has been allocated.

Executors

The screenshot shows the Apache Spark UI Executors tab. At the top, there's a summary table with metrics like Active(2), Dead(0), and Total(2) executors. Below it is a detailed Executors table listing two entries: one active executor with ID 0 and an 'driver' entry. The Executors table includes columns for Executor ID, Address, Status, RDD Blocks, Storage Memory, Disk Used, Cores, Resources, Active Tasks, Failed Tasks, Complete Tasks, Total Tasks, Task Time (GC Time), Input, Shuffle Read, Shuffle Write, and Logs. A red arrow points from the 'Resources' checkbox in the summary filters to the 'Logs' column in the Executors table.

RDD Blocks	Storage Memory	Disk Used	Cores	Active Tasks	Failed Tasks	Complete Tasks	Total Tasks	Task Time (GC Time)	Input	Shuffle Read	Shuffle Write	Blacklisted
Active(2) 0	0.0 B / 13 GiB	0.0 B	8	0	0	839	839	5.4 min (1 s)	2.8 GiB	1.2 GiB	1.2 GiB	0
Dead(0) 0	0.0 B / 0.0 B	0.0 B	0	0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	0
Total(2) 0	0.0 B / 13 GiB	0.0 B	8	0	0	839	839	5.4 min (1 s)	2.8 GiB	1.2 GiB	1.2 GiB	0

Executor ID	Address	Status	RDD Blocks	Storage Memory	Disk Used	Cores	Resources	Active Tasks	Failed Tasks	Complete Tasks	Total Tasks	Task Time (GC Time)	Input	Shuffle Read	Shuffle Write	Logs
0	10.19.183.153:45123	Active	0	0.0 B / 7.8 GiB	0.0 B	8	gpu: [1]	0	0	839	839	5.4 min (1 s)	2.8 GiB	1.2 GiB	1.2 GiB	stdout stderr
driver	spark-gashen:33965	Active	0	0.0 B / 5.2 GiB	0.0 B	0		0	0	0	0	0.0 ms (0.0 ms)	0.0 B	0.0 B	0.0 B	

Debugging

For now, the best way to debug is how you would normally do it on Spark. Look at the UI and log files to see what failed. If you have a seg fault from the GPU find the `hs_err_pid.log` file. To make sure your `hs_err_pid.log` file goes into the YARN application log directory, you can add in the config: `--conf spark.executor.extraJavaOptions="--XX:ErrorFile=<LOG_DIR>/hs_err_pid_%p.log"`.

If you want to see why an operation did not run on the GPU, turn on the configuration: `--conf spark.rapids.sql.explain=NOT_ON_GPU`. A log message is output to the Driver log as to why a Spark operation is not able to run on the GPU.

Out of GPU Memory

GPU out of memory can show up in multiple ways. You can see an out of memory error or it can also manifest as just crashes. Generally this means your partition size is too big, go back to the Configuration section for the partition size and/or the number of partitions. Possibly reduce the number of concurrent GPU tasks to one. The Spark UI may give you a hint at the size of the data. Look at either the input data or the shuffle data size for the stage that failed.

Summary

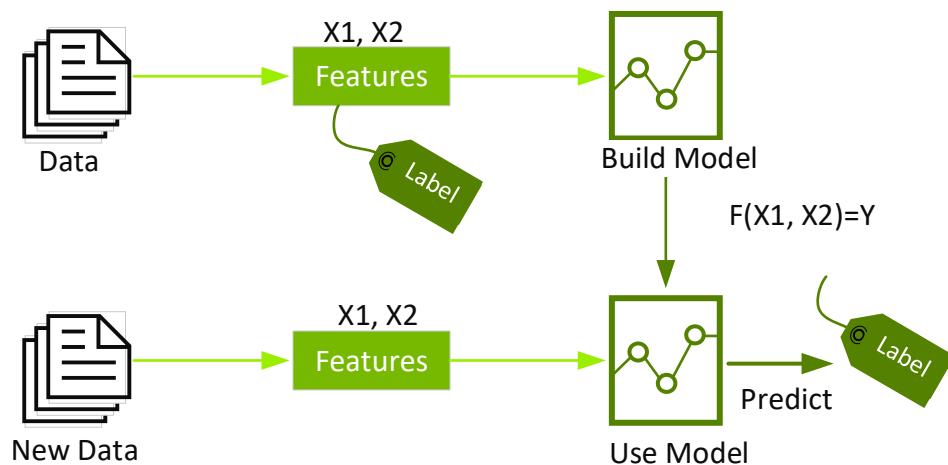
In this chapter, we covered the basics of getting started using the new RAPIDS APIs Plugin for Apache Spark 3.x that leverages GPUs to accelerate processing. For more information refer to the [RAPIDS Accelerator for Spark guide](#).

Chapter 5: Predicting Housing Prices Using Apache Spark Machine Learning

Zillow is one of the largest marketplaces for real estate information in the U.S. and a leading example of impactful machine learning (ML). [Zillow Research](#) uses ML models that analyze hundreds of data points on each property to estimate home values and predict market changes. In this chapter, we cover how to use Apache Spark ML Random Forest Regression to predict the median sales prices for homes in a region. Note that currently only XGBoost is GPU-Accelerated in Spark ML, which we will cover in the next chapter.

Classification and Regression

Classification and regression are two categories of supervised machine learning algorithms. Supervised ML, also called predictive analytics, uses algorithms to find patterns in labeled data and then uses a model that recognizes those patterns to predict the labels on new data. Classification and regression algorithms take a dataset with labels (also called the target outcome) and features (also called properties) and learn how to label new data based on those data features.



Classification identifies which category an item belongs to, such as whether a credit card transaction is legitimate. Regression predicts a continuous numeric value like a house price, for example.

Regression

Regression estimates the relationship between a target outcome dependent variable (the label) and one or more independent variables (the features). Regression can be used to analyze the strength of the relationship between the label and the feature variables, determine how much the label changes with an adjustment in one or more feature variables, and predict trends between the label and feature variables.

Let's go through a linear regression example of housing prices, given historical house prices and features of houses (square feet, number of bedrooms, location, etc.):

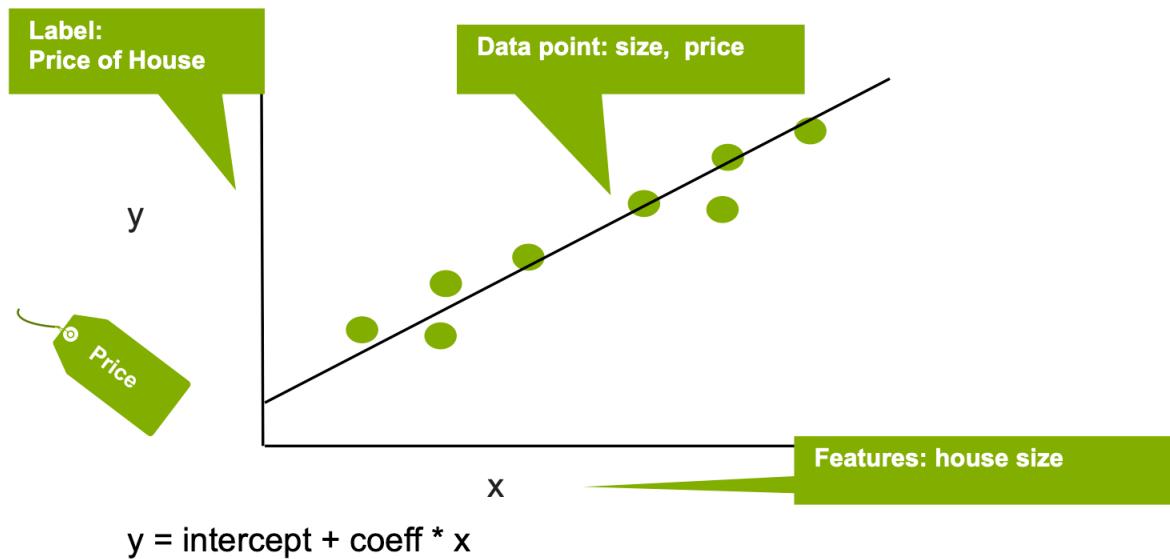
- ▶ What are we trying to predict?

This is the label: the house price

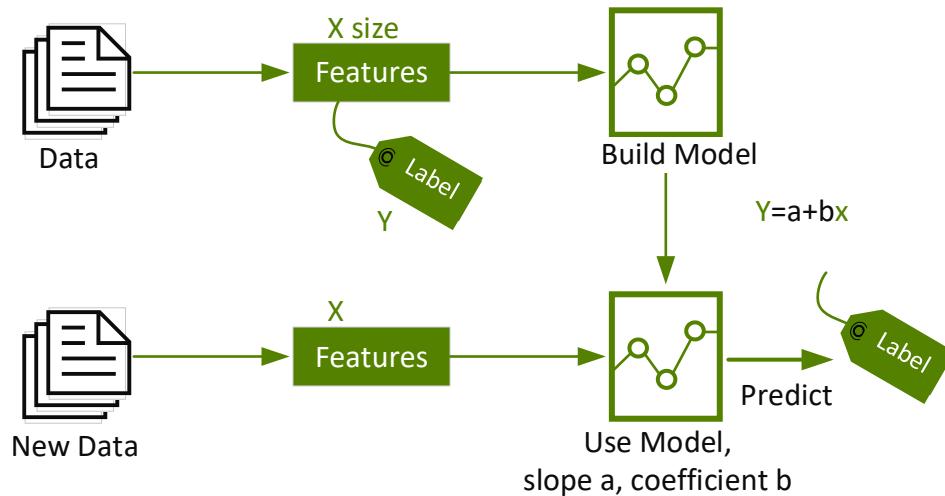
- ▶ What are the data properties that you can use to predict?

These are the features: to build a regression model, you extract the features of interest that have the strongest relationship with the label and contribute the most to the prediction.

In the following example, we'll use the size of the house.



Linear regression models the relationship between the Y "Label" and the X "Feature", in this case the relationship between the house price and size, with the equation: $Y = \text{intercept} + (\text{coefficient} * X) + \text{error}$. The coefficient measures the impact of the feature on the label, in this case the impact of the house size on the price.



Multiple linear regression models the relationship between two or more "Features" and a "Label." For example, if we wanted to model the relationship between the price and the house size, the number of bedrooms, and the number of bathrooms, the multiple linear regression function would look like this:

$$Y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

Price = intercept + (coefficient1 size) + (coefficient2 bedrooms) + (coefficient3 * bathrooms) + error.

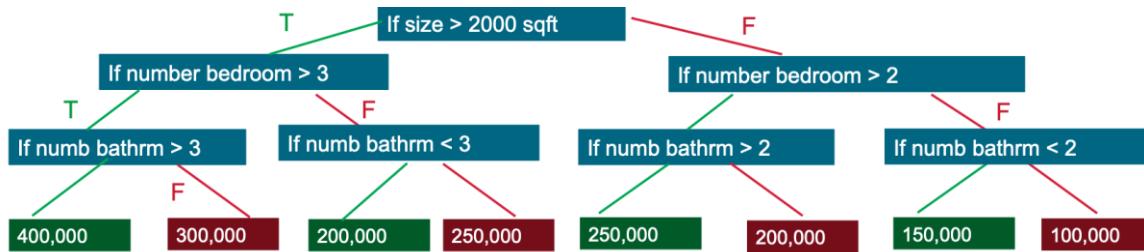
The coefficients measure the impact on the price of each of the features.

Decision Trees

Decision trees create a model that predicts the label by evaluating a set of rules that follow an if-then-else pattern. The if-then-else feature questions are the nodes, and the answers "true" or "false" are the branches in the tree to the child nodes.

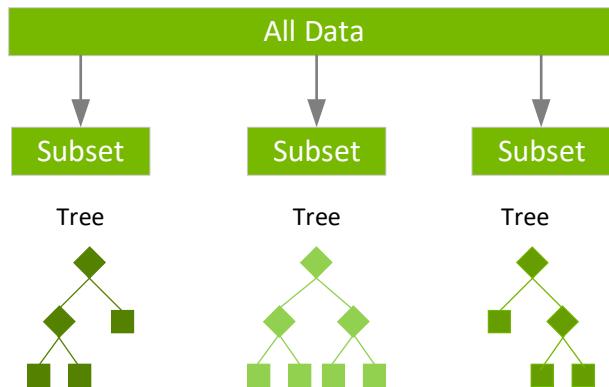
A decision tree model estimates the minimum number of true/false questions needed to assess the probability of making a correct decision. Decision trees can be used for classification to predict a category, or probability of a category, or regression to predict a continuous numeric value. Following is an example of a simplified decision tree to predict housing prices:

- ▶ Q1: If the size of the house > 2000sqft
 - T:Q2: If the number of bedrooms > 3
 - ▶ T:Q3: If the number of bathrooms is > 3
 - T: Price=\$400,000
 - F: Price=\$200,000



Random Forests

Ensemble learning algorithms combine multiple machine learning algorithms to obtain a better model. Random forest is a popular ensemble learning method for classification and regression. The algorithm builds a model consisting of multiple decision trees, based on different subsets of data at the training stage. Predictions are made by combining the output from all the trees, which reduces the variance and improves the predictive accuracy. For random forest classification, the label is predicted to be the class predicted by the majority of trees. For random forest regression, the label is the mean regression prediction of the individual trees.



Spark provides the following algorithms for regression:

- ▶ Linear regression
- ▶ Generalized linear regression
- ▶ Decision tree regression
- ▶ Random forest regression
- ▶ Gradient-boosted tree regression
- ▶ XGBoost regression
- ▶ Survival regression
- ▶ Isotonic regression

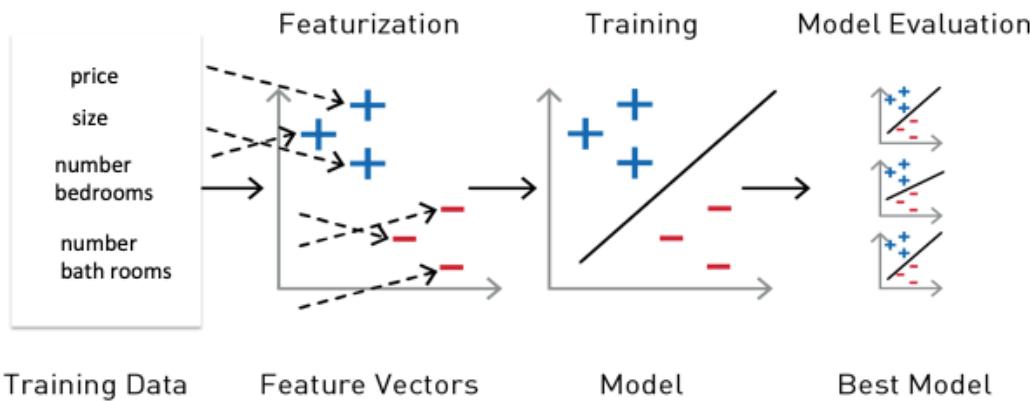
Machine Learning Workflows

Machine learning is an iterative process which involves:

- ▶ Extracting, Transforming, Loading (ETL) and analyzing historical data in order to extract the significant features and label.
- ▶ Training, testing, and evaluating the results of ML algorithms to build a model.
- ▶ Using the model in production with new data to make predictions.
- ▶ Model monitoring and model updating with new data.

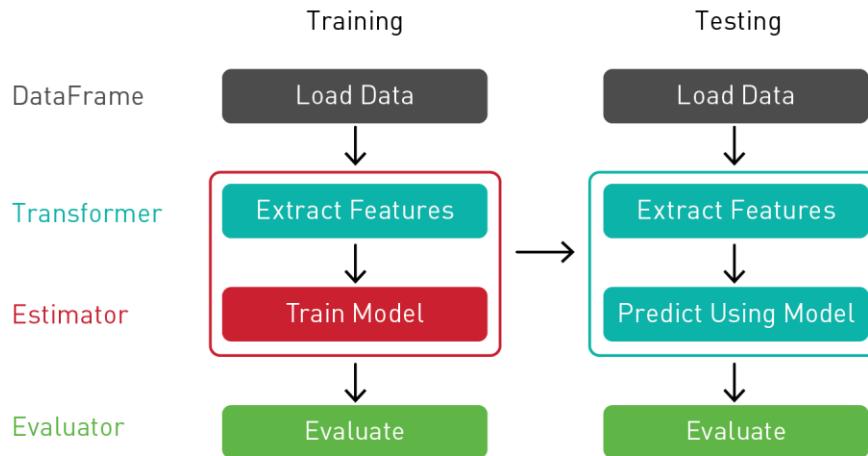
Using Spark ML Pipelines

For the features and label to be used by an ML algorithm, they must be put into a feature vector, which is a vector of numbers representing the value for each feature. Feature vectors are used to train, test, and evaluate the results of an ML algorithm to build the best model.



Reference Learning Spark

Spark ML provides a uniform set of high-level APIs, built on top of DataFrames for building ML pipelines or workflows. Having ML pipelines built on top of DataFrames provides the scalability of partitioned data processing with the ease of SQL for data manipulation.



We use a Spark ML Pipeline to pass the data through transformers and extract the features, an estimator to produce the model, and an evaluator to measure the accuracy of the model.

- ▶ **Transformer:** A Transformer is an algorithm that transforms one DataFrame into another DataFrame. We'll use a Transformer to create a DataFrame with a features vector column.
- ▶ **Estimator:** An Estimator is an algorithm that can be fit on a DataFrame to produce a transformer. We'll use an estimator to train a model, and return a model Transformer, which can add a predictions column to a DataFrame with a features vector column.
- ▶ **Pipeline:** A pipeline chains multiple Transformers and Estimators together to specify an ML workflow.
- ▶ **Evaluator:** An Evaluator measures the accuracy of a trained Model on label and prediction DataFrame columns.

Example Use Case Dataset

In this example, we'll be using the California housing prices dataset from the [StatLib repository](#). This dataset contains 20,640 records based on data from the 1990 California census, with each record representing a geographic block. The following list provides a description for the attributes of the data set.

- ▶ **Median House Value:** Median house value (in thousands of dollars) for households within a block.
- ▶ **Longitude:** East/west measurement, a higher value is further west.
- ▶ **Latitude:** North/south measurement, a higher value is further north.
- ▶ **Housing Median Age:** Median age of a house within a block, lower is newer.
- ▶ **Total Rooms:** Total number of rooms within a block.
- ▶ **Total Bedrooms:** Total number of bedrooms within a block.
- ▶ **Population:** Total number of people residing within a block.
- ▶ **Households:** Total number of households in a block.
- ▶ **Median Income:** Median income for households within a block of houses (measured in tens of thousands of dollars).

To build a model, you extract the features that most contribute to the prediction. In order to make some of the features more relevant for predicting the median house value, instead of using totals we'll calculate and use these ratios: rooms per house=total rooms/households, people per house=population/households, and bedrooms per room=total bedrooms/total rooms.

In this scenario, we use random forest regression on the following label and features:

- ▶ Label → median house value
- ▶ Features → {"median age", "median income", "rooms per house", "population per house", "bedrooms per room", "longitude", "latitude" }

Load the Data from a File into a DataFrame



The first step is to load our data into a DataFrame. In the following code, we specify the data source and schema to load into a dataset.

```
import org.apache.spark._  
import org.apache.spark.ml._  
import org.apache.spark.ml.feature._  
import org.apache.spark.ml.regression._  
import org.apache.spark.ml.evaluation._  
import org.apache.spark.ml.tuning._
```

```

import org.apache.spark.sql._
import org.apache.spark.sql.functions._
import org.apache.spark.sql.types._
import org.apache.spark.ml.Pipeline

val schema = StructType(Array(
    StructField("longitude", FloatType, true),
    StructField("latitude", FloatType, true),
    StructField("medage", FloatType, true),
    StructField("totalrooms", FloatType, true),
    StructField("totalbdrms", FloatType, true),
    StructField("population", FloatType, true),
    StructField("houshlds", FloatType, true),
    StructField("medincome", FloatType, true),
    StructField("medhvalue", FloatType, true)
))

var file ="/path/cal_housing.csv"

var df = spark.read.format("csv").option("inferSchema", "false").schema(schema).load(file)

df.show
result:
+-----+-----+-----+-----+-----+-----+-----+
|longitude|latitude|medage|totalrooms|totalbdrms|population|houshlds|medincome|medhvalue|
+-----+-----+-----+-----+-----+-----+-----+
| -122.23| 37.88| 41.0| 880.0| 129.0| 322.0| 126.0| 8.3252| 452600.0|
| -122.22| 37.86| 21.0| 7099.0| 1106.0| 2401.0| 1138.0| 8.3014| 358500.0|
| -122.24| 37.85| 52.0| 1467.0| 190.0| 496.0| 177.0| 7.2574| 352100.0|
+-----+-----+-----+-----+-----+-----+-----+

```

In the following code example, we use the DataFrame withColumn() transformation, to add columns for the ratio features: rooms per house=total rooms/households, people per house=population/households, and bedrooms per rooms=total bedrooms/total rooms. We then cache the DataFrame and create a temporary view for better performance and ease of using SQL.

```

// create ratios for features
df = df.withColumn("roomsPhouse", col("totalrooms")/col("houshlds"))
df = df.withColumn("popPhouse", col("population")/col("houshlds"))
df = df.withColumn("bedrmsPRoom", col("totalbdrms")/col("totalrooms"))

df=df.drop("totalrooms", "houshlds", "population", "totalbdrms")

df.cache
df.createOrReplaceTempView("house")
spark.catalog.cacheTable("house")

```

Summary Statistics

Spark DataFrames include some [built-in functions](#) for statistical processing. The `describe()` function performs summary statistics calculations on numeric columns and returns them as a DataFrame. The following code shows some statistics for the label and some features.

```
df.describe("medincome","medhvalue","roomsPhouse","popPhouse").show

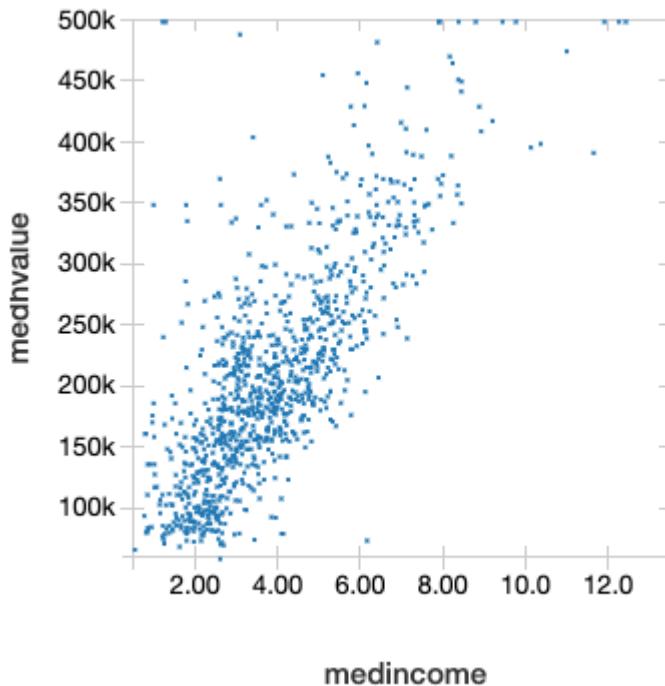
result:
+-----+-----+-----+-----+
|summary| medincome | medhvalue | roomsPhouse | popPhouse |
+-----+-----+-----+-----+
| count | 20640 | 20640 | 20640 | 20640 |
| mean | 3.8706710030346416 | 206855.81690891474 | 5.428999742190365 | 3.070655159436382 |
| stddev | 1.8998217183639696 | 115395.61587441359 | 2.4741731394243205 | 10.38604956221361 |
| min | 0.4999 | 14999.0 | 0.8461538461538461 | 0.6923076923076923 |
| max | 15.0001 | 500001.0 | 141.9090909090909 | 1243.333333333333 |
+-----+-----+-----+-----+
```

The DataFrame `Corr()` function calculates the Pearson correlation coefficient of two columns of a DataFrame. This measures the statistical relationship between two variables based on the method of covariance. Correlation coefficient values range from 1 to -1, where 1 indicates a perfect positive relationship, -1 indicates a perfect negative relationship, and a 0 indicates no relationship. Below we see that the median income and the median house value have a positive correlation relationship.

```
df.select(corr("medhvalue","medincome")).show()

+-----+
| corr(medhvalue, medincome) |
+-----+
| 0.688075207464692 |
+-----+
```

The following scatterplot of the median house value on the Y axis and median income on the X axis shows that they are linearly related to each other.



The following code uses the DataFrame randomSplit method to randomly split the Dataset into two, with 80% for training and 20% for testing.

```
val Array(trainingData, testData) = df.randomSplit(Array(0.8, 0.2), 1234)
```

Feature Extraction and Pipelining

The following code creates a VectorAssembler (a transformer), which will be used in a pipeline to combine a given list of columns into a single feature vector column.

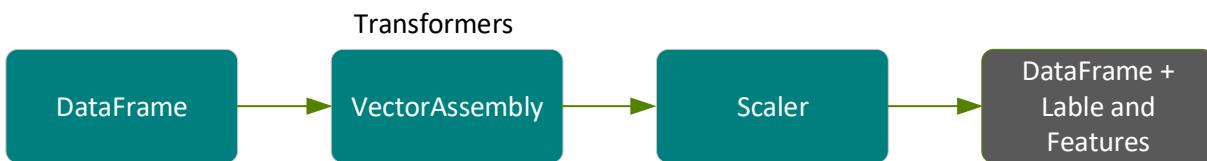
```
val featureCols = Array("medage", "medincome", "roomsPhouse", "popPhouse",
"bedrmsPRoom", "longitude", "latitude")

//put features into a feature vector column
val assembler = new
VectorAssembler().setInputCols(featureCols).setOutputCol("rawfeatures")
```

The following code creates a `StandardScaler` (a transformer), which will be used in a pipeline to standardize features by scaling to unit variance using DataFrame column summary statistics.

```
val scaler = new StandardScaler().setInputCol("rawfeatures").setOutputCol("features").setWithStd(true).setWithMean(true)
```

The result of running these transformers in a pipeline will be to add a scaled features column to the dataset as shown in the following figure.



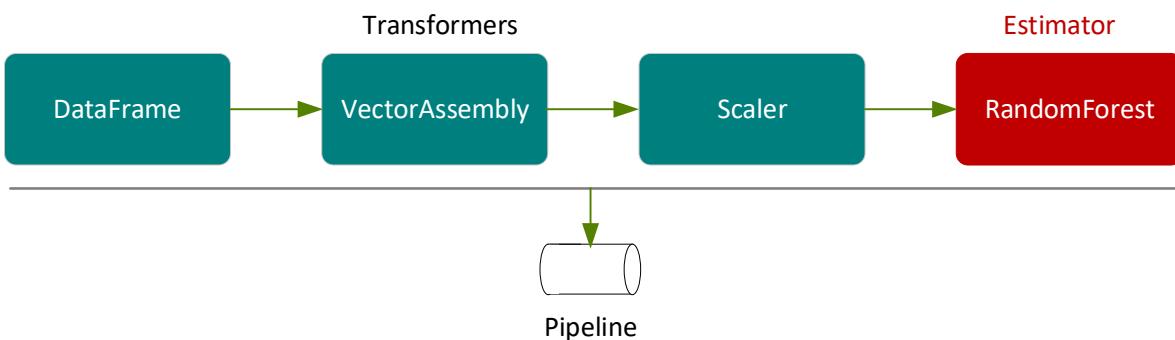
The final element in our pipeline is a `RandomForestRegressor` (an estimator), which trains on the vector of features and label, and then return a `RandomForestRegressorModel` (a transformer).

```
val rf = new RandomForestRegressor().setLabelCol("medhvalue").setFeaturesCol("features")
```

In the following example, we put the `VectorAssembler`, `Scaler` and `RandomForestRegressor` in a `Pipeline`. A pipeline chains multiple transformers and estimators together to specify an ML workflow for training and using a model.

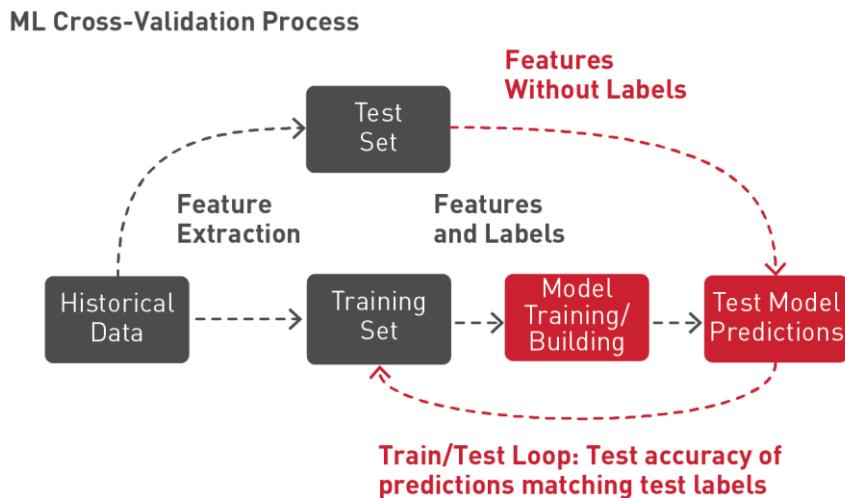
```
val steps = Array(assembler, scaler, rf)

val pipeline = new Pipeline().setStages(steps)
```

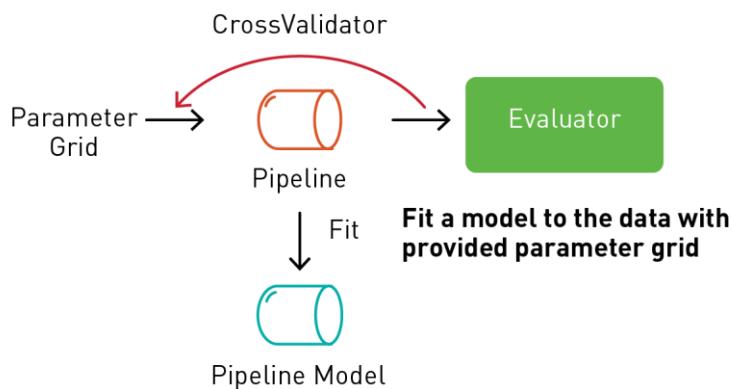


Train the Model

Spark ML supports a technique called k-fold cross-validation to try out different combinations of parameters in order to determine which parameter values of the ML algorithm produce the best model. With k-fold cross-validation, the data is randomly split into k partitions. Each partition is used once as the test dataset, while the rest are used for training. Models are then generated using the training sets and evaluated with the testing sets, resulting in k model accuracy measurements. The model parameters leading to the highest accuracy measurements produce the best model.



Spark ML supports k-fold cross-validation with a transformation/estimation pipeline which tries out different combinations of parameters, using a process called grid search, where you set up the parameters to test in a cross-validation workflow.



```
val cvModel = crossval.fit(ntrain)
```

The following code uses a `ParamGridBuilder` to construct the parameter grid for the model training. We define a `RegressionEvaluator`, which will evaluate the model by comparing the test `medhvalue` column with the test prediction column. We use a `CrossValidator` for model selection. The `CrossValidator` uses the pipeline, the parameter grid, and the evaluator to fit the training dataset and return the best model. The `CrossValidator` uses the `ParamGridBuilder` to iterate through the `maxDepth`, `maxBins`, and `numTrees` parameters of the `RandomForestRegressor` estimator and to evaluate the models, repeating three times per parameter value for reliable results.

```
val paramGrid = new ParamGridBuilder()
    .addGrid(rf.maxBins, Array(100, 200))
    .addGrid(rf.maxDepth, Array(2, 7, 10))
    .addGrid(rf.numTrees, Array(5, 20))
    .build()

val evaluator = new RegressionEvaluator()
    .setLabelCol("medhvalue")
    .setPredictionCol("prediction")
    .setMetricName("rmse")

val crossvalidator = new CrossValidator()
    .setEstimator(pipeline)
    .setEvaluator(evaluator)
    .setEstimatorParamMaps(paramGrid)
    .setNumFolds(3)

// fit the training data set and return a model
val pipelineModel = crossvalidator.fit(trainingData)
```

Next, we can get the best model in order to print out the feature importances. The results show that the median income, population per house, and the longitude are the most important features.

```
val featureImportances = pipelineModel
    .bestModel.asInstanceOf[PipelineModel]
    .stages(2)
    .asInstanceOf[RandomForestRegressionModel]
    .featureImportances

assembler.getInputCols
    .zip(featureImportances.toArray)
    .sortBy(-_._2)
    .foreach { case (feat, imp) =>
        println(s"feature: $feat, importance: $imp") }

result:
```

```
feature: medincome, importance: 0.4531355014139285
feature: popPhouse, importance: 0.12807843645878508
feature: longitude, importance: 0.10501162983981065
feature: latitude, importance: 0.1044621179898163
feature: bedrmsPRoom, importance: 0.09720295935509805
feature: roomsPhouse, importance: 0.058427239343697555
feature: medage, importance: 0.05368211559886386
```

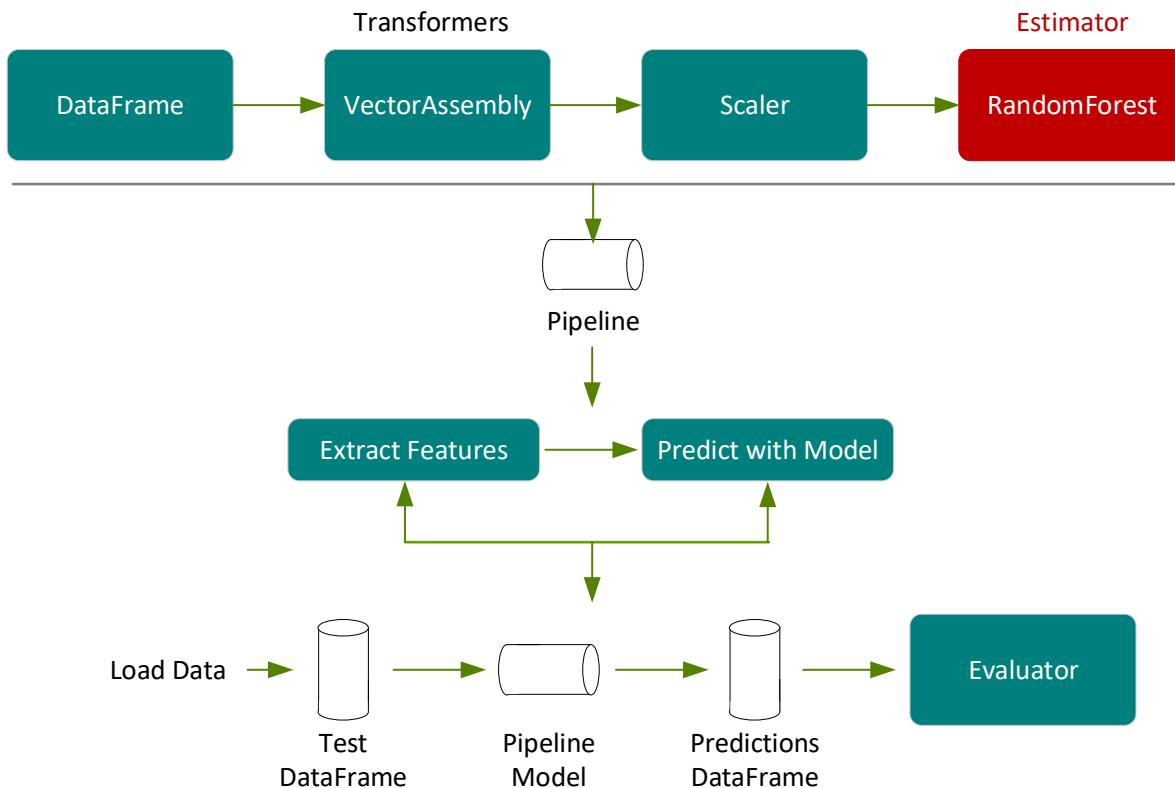
In the following example we get the parameters for the best random forest model produced, using the cross-validation process, which returns: max depth of 2, max bins of 50 and 5 trees.

```
val bestEstimatorParamMap = pipelineModel
    .getEstimatorParamMaps
    .zip(pipelineModel.avgMetrics)
    .maxBy(_._2)
    ._1
println(s"Best params:\n$bestEstimatorParamMap")

result:
rfr_maxBins: 50,
rfr_maxDepth: 2,
rfr_numTrees: 5
```

Predictions and Model Evaluation

Next we use the test DataFrame, which was a 20% random split of the original DataFrame, and was not used for training, to measure the accuracy of the model.

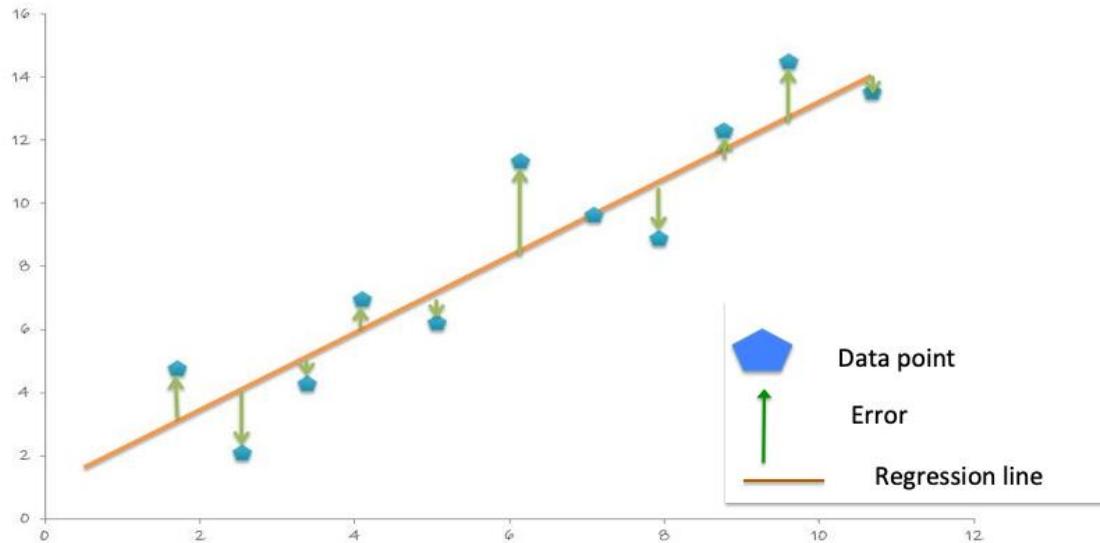


In the following code we call transform on the pipeline model, which will pass the test DataFrame, according to the pipeline steps, through the feature extraction stage, estimate with the random forest model chosen by model tuning, and then return the predictions in a column of a new DataFrame.

```
val predictions = pipelineModel.transform(testData)
predictions.select("prediction", "medhvalue").show(5)
```

```
result:
+-----+-----+
|      prediction|medhvalue|
+-----+-----+
|104349.59677450571| 94600.0 |
| 77530.43231856065| 85800.0 |
|111369.71756877871| 90100.0 |
| 97351.87386020401| 82800.0 |
+-----+-----+
```

With the predictions and labels from the test data, we can now evaluate the model. To evaluate the linear regression model, you measure how close the predictions values are to the label values. The error in a prediction, shown by the green lines below, is the difference between the prediction (the regression line Y value) and the actual Y value, or label. (Error = prediction - label).



The Mean Absolute Error (MAE) is the mean of the absolute difference between the label and the model's predictions. The absolute removes any negative signs.

$$\text{MAE} = \frac{\text{sum}(\text{absolute}(\text{prediction}-\text{label}))}{\text{number of observations}}$$

The Mean Square Error (MSE) is the sum of the squared errors divided by the number of observations. The squaring removes any negative signs and also gives more weight to larger differences. (MSE = $\frac{\text{sum}(\text{squared}(\text{prediction}-\text{label}))}{\text{number of observations}}$).

The Root Mean Squared Error (RMSE) is the square root of the MSE. RMSE is the standard deviation of the prediction errors. The Error is a measure of how far from the regression line label data points are and RMSE is a measure of how spread out these errors are.

The following code example uses the DataFrame `withColumn` transformation, to add a column for the error in prediction: `error=prediction-medhvalue`. Then we display the summary statistics for the prediction, the median house value, and the error (in thousands of dollars).

```
predictions = predictions.withColumn("error", col("prediction")-
    col("medhvalue"))

predictions.select("prediction", "medhvalue", "error").show

result:
+-----+-----+-----+
|      prediction|medhvalue|      error|
+-----+-----+-----+
| 104349.5967745057| 94600.0| 9749.596774505713|
```

```
| 77530.4323185606| 85800.0| -8269.567681439352|
| 101253.3225967887| 103600.0| -2346.677403211302|
+-----+-----+-----+
```



```
predictions.describe("prediction", "medhvalue", "error").show
result:
+-----+-----+-----+
|summary|      prediction|      medhvalue|      error|
+-----+-----+-----+
|  count|          4161|          4161|          4161|
|  mean|206307.4865123929|205547.72650805095| 759.7600043416329|
| stddev|97133.45817381598|114708.03790345002| 52725.56329678355|
|  min|56471.09903814694|        26900.0|-339450.5381565819|
|  max|499238.1371374392|        500001.0|293793.71945819416|
+-----+-----+-----+
```

The following code example uses the Spark RegressionEvaluator to calculate the MAE on the predictions DataFrame, which returns 36636.35 (in thousands of dollars).

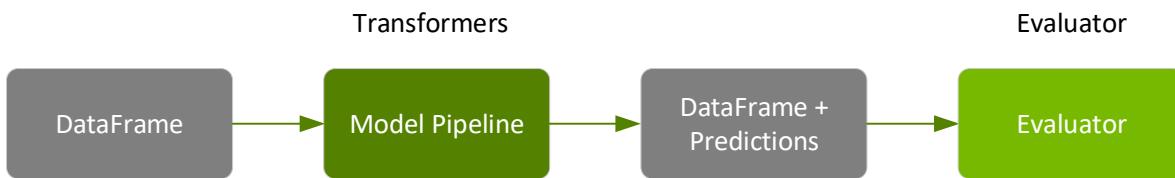
```
val maevaluator = new RegressionEvaluator()
  .setLabelCol("medhvalue")
  .setMetricName("mae")

val mae = maevaluator.evaluate(predictions)
result:
mae: Double = 36636.35
```

The following code example uses the Spark RegressionEvaluator to calculate the RMSE on the predictions DataFrame, which returns 52724.70.

```
val evaluator = new RegressionEvaluator()
  .setLabelCol("medhvalue")
  .setMetricName("rmse")
val rmse = evaluator.evaluate(predictions)

result:
rmse: Double = 52724.70
```



Save the Model

We can now save our fitted pipeline model to the distributed file store for later use in production. This saves both the feature extraction stage and the random forest model chosen by model tuning.

```
pipelineModel.write.overwrite().save(modeldir)
```

The result of saving the pipeline model is a JSON file for metadata and a Parquet for model data. We can reload the model with the load command; the original and reloaded models are the same:

```
val sameModel = CrossValidatorModel.load("modeldir")
```

Summary

In this chapter, we discussed Regression, Decision Trees, and Random Forest algorithms. We covered the fundamentals of Spark ML pipelines and worked through a real world example to predict median house prices.

Chapter 6: Predicting Taxi Fares Using GPU-Accelerated XGBoost

Big data is [one of the 10 major areas](#) used to improve cities. The analysis of location and behavior patterns within cities allows for optimization of traffic, better planning decisions, and smarter advertising. For example, the analysis of GPS car data enables cities to optimize traffic flows based on real-time traffic information. Telecom companies are using mobile phone location data to provide insights by identifying and predicting the location activity trends and patterns of a population in large metropolitan areas. And, the application of machine learning (ML) to geolocation data is proving instrumental in identifying patterns and trends for the telecom, travel, marketing, and manufacturing industries.

In this chapter, we'll use public New York Taxi trip data to examine regression analysis on taxi trip data as it pertains to predicting NYC taxi fares. We'll start with an overview of the XGBoost algorithm and then explore the use case.

XGBoost

[XGBoost](#), which stands for Extreme Gradient Boosting, is a scalable, distributed [gradient-boosted](#) decision tree (GBDT) machine learning library. XGBoost provides parallel tree boosting and is the leading ML library for regression, classification, and ranking problems. The RAPIDS team works closely with the Distributed Machine Learning Common (DMLC) XGBoost organization, and XGBoost now includes seamless, drop-in GPU acceleration, significantly speeding up model training and improving accuracy for better predictions.

Gradient Boosting Decision Trees (GBDTs) is a decision tree ensemble algorithm similar to Random Forest, the difference is in how the trees are built and combined. Random Forest uses a technique called bagging to build full decision trees in parallel from bootstrap samples of the data set. The final prediction is an average of all of the decision tree predictions. Gradient Boosting Decision Trees use a technique called boosting to iteratively train an ensemble of shallow decision trees, with each iteration using weights given to records in the previous sample, which did not predict correctly, to decrease the error of the succeeding tree. The final prediction is a weighted average of all of the decision tree predictions. Bagging minimizes the variance and overfitting, boosting minimizes the bias and underfitting.

XGBoost is a variation of GBDTs. With GBDTs, the decision trees are built sequentially. With XGBoost, trees are built in parallel, following a level-wise strategy, scanning across gradient values and using these partial sums to evaluate the quality of splits at every possible split in the training set.

GPU-Accelerated XGBoost

The [GPU-accelerated XGBoost](#) algorithm makes use of fast parallel prefix sum operations to scan through all possible splits, as well as parallel radix sorting to repartition data. It builds a decision tree for a given boosting iteration, one level at a time, processing the entire Dataset concurrently on the GPU.

GPU-accelerated Spark XGBoost offers the following [key features](#):

- ▶ **Partitioning of ORC, CSV, and Parquet input files across multi GPUs**
Essentially any number/size of supported input file formats can be divided up evenly among the different training nodes.
- ▶ **GPU-accelerated training**
Improved XGBoost training time with a dynamic in-memory representation of the training data that optimally stores features based on the sparsity of a dataset rather than a fixed in-memory representation based on the largest number of features amongst different training instances. Decision trees are built using gradient pairs that can be reused to save memory, reducing copies to increase performance.
- ▶ **Efficient GPU memory utilization**
XGBoost requires data to fit into memory which creates a restriction on data size using either a single GPU or distributed multi-GPU multi-node training. Now, with improved GPU memory utilization, users can train with five times the size of data as compared to the first version. This is one of the critical factors to improve total cost of training without impacting performance.

Example Use Case Dataset

The example dataset is a [New York Taxi Dataset](#), which has already been cleaned up and transformed to add features, such as the [haversine distance](#) using this [Spark ETL notebook](#).

In this scenario, we'll build a model to predict the taxi fare amount, based on the following features:

- ▶ **Label → fare amount**
- ▶ **Features → {passenger count, trip distance, pickup longitude, pickup latitude, rate code, dropoff longitude, dropoff latitude, hour, day of week, is weekend}**

Load the Data from a File into a DataFrame

First, we import the packages needed for both GPU version and CPU versions of Spark xgboost:

```
import org.apache.spark.sql.functions._  
import org.apache.spark.sql.types._  
import org.apache.spark.sql._  
import org.apache.spark.ml._  
import org.apache.spark.ml.feature._  
import org.apache.spark.ml.evaluation._  
import org.apache.spark.sql.types._  
import ml.dmlc.xgboost4j.scala.spark.{XGBoostRegressor,  
XGBoostRegressionModel}
```

For the GPU version of Spark xgboost you also need the following import:

```
import ml.dmlc.xgboost4j.scala.spark.rapids.{GpuDataReader, GpuDataset}
```

We specify the schema with a Spark [StructType](#).

```
lazy val schema =  
  StructType(Array(  
    StructField("vendor_id", DoubleType),  
    StructField("passenger_count", DoubleType),  
    StructField("trip_distance", DoubleType),  
    StructField("pickup_longitude", DoubleType),  
    StructField("pickup_latitude", DoubleType),  
    StructField("rate_code", DoubleType),  
    StructField("store_and_fwd", DoubleType),  
    StructField("dropoff_longitude", DoubleType),  
    StructField("dropoff_latitude", DoubleType),  
    StructField(labelName, DoubleType),  
    StructField("hour", DoubleType),  
    StructField("year", IntegerType),  
    StructField("month", IntegerType),  
    StructField("day", DoubleType),  
    StructField("day_of_week", DoubleType),  
    StructField("is_weekend", DoubleType)  
  ))
```

In the following code we create a Spark session and set the training and evaluation data file paths. (Note: If you are using a notebook, then you do not have to create the `SparkSession`.)

```
val trainPath = "/FileStore/tables/taxi_tsmall.csv"  
val evalPath  = "/FileStore/tables/taxi_esmall.csv"  
val spark = SparkSession.builder().appName("Taxi-GPU").getOrCreate
```

We load the data from a CSV file into a Spark DataFrame, specifying the datasource and schema to load into a DataFrame, as shown below.

Load Data → DataFrame

```
val tdf = spark.read.option("inferSchema",
"false").option("header", true).schema(schema).csv(trainPath)
val edf = spark.read.option("inferSchema", "false").option("header",
true).schema(schema).csv(evalPath)
```

DataFrame `show(5)` displays the first 5 rows:

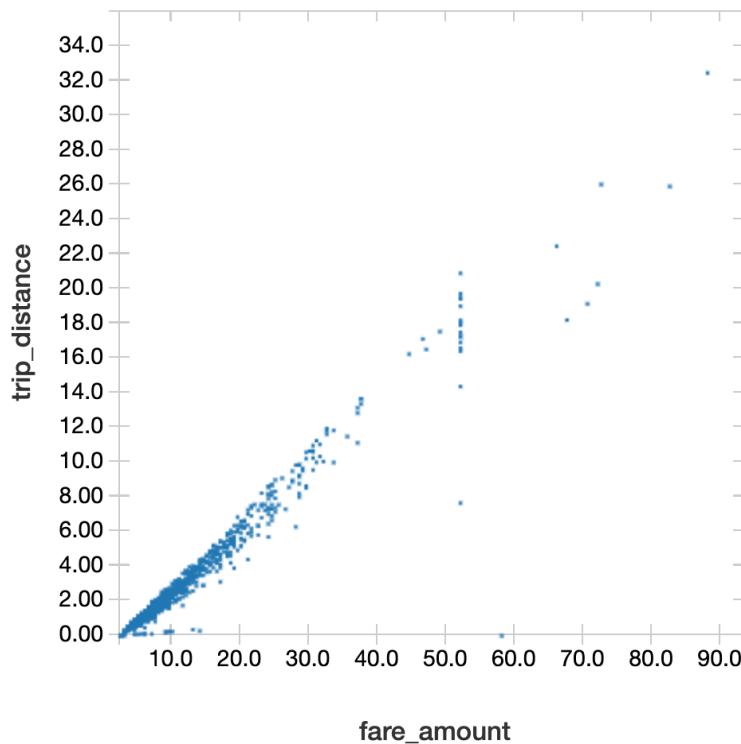
```
tdf.select("trip_distance", "rate_code", "fare_amount").show(5)
result:
+-----+-----+-----+
| trip_distance | rate_code | fare_amount |
+-----+-----+-----+
| 2.72 | -6.77418915E8 | 11.5 |
| 0.94 | -6.77418915E8 | 5.5 |
| 3.63 | -6.77418915E8 | 13.0 |
| 11.86 | -6.77418915E8 | 33.5 |
| 3.03 | -6.77418915E8 | 11.0 |
+-----+-----+-----+
```

The function `describe` returns a DataFrame containing descriptive summary statistics, such as count, mean, standard deviation, and minimum and maximum value for each numerical column.

```
tdf.select("trip_distance", "rate_code", "fare_amount").describe().show
+-----+-----+-----+
|summary| trip_distance | rate_code | fare_amount |
+-----+-----+-----+
| count | 7999 | 7999 | 7999 |
| mean | 3.278923615451919 | -6.569284350812602E8 | 12.348543567945994 |
| stddev | 3.6320775770793547 | 1.6677419425906155E8 | 10.221929466939088 |
| min | 0.0 | -6.77418915E8 | 2.5 |
| max | 35.97000000000006 | 1.957796822E9 | 107.5 |
+-----+-----+-----+
```

The following scatter plot is used to explore the correlation between the fare amount and the trip distance.

```
%sql
select trip_distance, fare_amount
from taxi
```



Define Features Array

For the features to be used by an ML algorithm, they are transformed and put into feature vectors, which are vectors of numbers representing the value for each feature. Below, a VectorAssembler transformer is used to return a new DataFrame with a label and a vector features column.



```
// feature column names
val featureNames = Array("passenger_count", "trip_distance",
"pickup_longitude", "pickup_latitude", "rate_code", "dropoff_longitude",
"dropoff_latitude", "hour", "day_of_week", "is_weekend")
// create transformer
object Vectorize {
```

```

def apply(df: DataFrame, featureNames: Seq[String], labelName: String):
DataFrame = {
    val toFloat = df.schema.map(f => col(f.name).cast(FloatType))
    new VectorAssembler()
        .setInputCols(featureNames.toArray)
        .setOutputCol("features")
        .transform(df.select(toFloat:_*))
        .select(col("features"), col(labelName))
}
}

// transform method adds features column
var trainSet = Vectorize(tdf, featureNames, labelName)
var evalSet = Vectorize(edf, featureNames, labelName)
trainSet.take(1)
result:
res8: Array[org.apache.spark.sql.Row] = Array([[5.0,2.7200000286102295,-
73.94813537597656,40.82982635498047,-6.77418944E8,-
73.96965026855469,40.79747009277344,10.0,6.0,1.0],11.5])

```

When using the XGBoost GPU version, the VectorAssembler is not needed.

For the CPU version the `num_workers` should be set to the number of CPU cores, the `tree_method` to "hist," and the features column to the output features column in the Vector Assembler.



```

lazy val paramMap = Map(
    "learning_rate" -> 0.05,
    "max_depth" -> 8,
    "subsample" -> 0.8,
    "gamma" -> 1,
    "num_round" -> 500
)
// set up xgboost parameters
val xgbParamFinal = paramMap ++ Map("tree_method" -> "hist", "num_workers" -> 12)
// create the xgboostregressor estimator
val xgbRegressor = new XGBoostRegressor(xgbParamFinal)
    .setLabelCol(labelName)
    .setFeaturesCol("features")

```

For the GPU version the `num_workers` should be set to the number of machines with GPU in the Spark cluster, the `tree_method` to “`gpu_hist`,” and the features column to an array of strings containing the feature names.

```
val xgbParamFinal = paramMap ++ Map("tree_method" -> "gpu_hist",
"num_workers" -> 1)
// create the estimator
val xgbRegressor = new XGBoostRegressor(xgbParamFinal)
.setLabelCol(labelName)
.setFeaturesCols(featureNames)
```

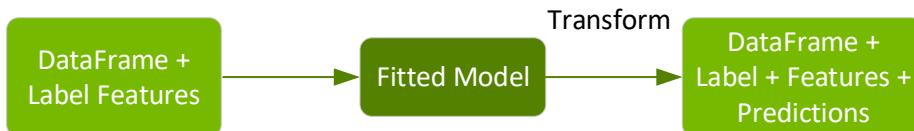
The following code uses the `XGBoostRegressor` estimator `fit` method on the training dataset to train and return an `XGBoostRegressor` model. We also use a `time` method to return the time to train the model and we use this to compare the time training with CPU vs. GPU.



```
object Benchmark {
  def time[R](phase: String)(block: => R): (R, Float) = {
    val t0 = System.currentTimeMillis
    val result = block // call-by-name
    val t1 = System.currentTimeMillis
    println("Elapsed time [" + phase + "]: " +
      ((t1 - t0).toFloat / 1000) + "s")
    (result, (t1 - t0).toFloat / 1000)
  }
}
// use the estimator to fit (train) a model
val (model, _) = Benchmark.time("train") {
  xgbRegressor.fit(trainSet)
}
```

The performance of the model can be evaluated using the eval dataset which has not been used for training. We get predictions on the test data using the model transform method.

The model will estimate with the trained XGBoost model, and then return the fare amount predictions in a new predictions column of the returned DataFrame. Here again, we use the Benchmark time method in order to compare prediction times.



```

val (prediction, _) = Benchmark.time("transform") {
  val ret = model.transform(evalSet).cache()
  ret.foreachPartition(_ => ())
  ret
}

prediction.select( labelName, "prediction").show(10)
Result:
+-----+-----+
|fare_amount|      prediction|
+-----+-----+
|      5.0| 4.749197959899902|
|     34.0|38.651187896728516|
|    10.0|11.101678848266602|
|    16.5| 17.23284912109375|
|     7.0| 8.149757385253906|
|     7.5|7.5153608322143555|
|     5.5| 7.248467922210693|
|     2.5|12.289423942565918|
|     9.5|10.893491744995117|
|    12.0| 12.06682014465332|
+-----+-----+
  
```

The [RegressionEvaluator](#) evaluate method calculates the root mean square error, which is the square root of the mean squared error, from the prediction and label columns.



```

val evaluator = new RegressionEvaluator().setLabelCol(labelName)
val (rmse, _) = Benchmark.time("evaluation") {
  evaluator.evaluate(prediction)
}
println(s"RMSE == $rmse")
Result:
Elapsed time [evaluation]: 0.356s
RMSE == 2.6105287283128353
  
```

Save the Model

The model can be saved to disk, as shown below, in order to use later.

```
model.write.overwrite().save(savepath)
```

The result of saving the model is a JSON file for metadata and a Parquet file for model data. We can reload the model with the load command. The original and reloaded models are the same.

```
val sameModel = XGBoostRegressionModel.load(savepath)
```

Summary

In this chapter, we covered the basics of how XGBoost works and how to use XGBoost Regression with Spark to predict taxi fare amounts. You can now run this example on CPUs and GPUs with a larger dataset to compare time and accuracy of predictions.

Appendex: Code

Code

You can download the code to run the examples in the book from here:

- ▶ <https://github.com/caroljmcDonald/spark3-book>
- ▶ <https://github.com/rapidsai/spark-examples>

Additional Resources

- ▶ Spark documentation including deployment and configuration:
<https://spark.apache.org/docs/latest/>
- ▶ RAPIDS Accelerator for Spark
<https://nvidia.github.io/spark-rapids/>
- ▶ RAPIDS AI home <https://rapids.ai/>
- ▶ NVIDIA Developer portal <https://developer.nvidia.com/>

About the Author

Carol has experience in many roles including software architecture/development, training, technology evangelism, and developer outreach. As a Solutions Architect and Instructor at MapR, Carol focused on big data, Apache Spark, Apache HBase, Apache Drill, and machine learning in healthcare, finance, and telecom. As a Java Technology Evangelist at Sun, Carol traveled worldwide, speaking, and giving Hands-on-Labs at Sun Tech Days. As a software developer and architect, Carol developed complex mission-critical applications in the banking, health insurance and telecom industries including: a large health information exchange connecting over one million providers and health plans, a large loan servicing application for Wells Fargo, Drug Development Intranet applications for Hoffman La Roche, Telecom Network Management applications for HP, Open Systems Interconnection messaging applications for IBM, and Sigint applications for the NSA. Carol holds an MS in computer science from the University of Tennessee and a BS in geology from Vanderbilt University and is an O'Reilly Certified Spark Developer, MapR certified Spark and HBase developer, and Sun Certified Java Architect and Java Programmer. Carol is fluent in English, French, and German.

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