databricks

Big Book of Machine Learning Use Cases

03 EDITION

Contents

CHAPTER 1:

Introduction

Organizations across many industries are using machine learning to power new customer experiences, optimize business processes and improve employee productivity. From detecting financial fraud to improving the play-by-play decision-making for professional sports teams, this book brings together a multitude of practical use cases to get you started on your machine learning journey. The collection also serves as a guide — including code samples and notebooks — so you can roll up your sleeves and dive into machine learning on the Databricks Lakehouse.

CHAPTER 2:

Moneyball 2.0: Improving Pitch-by-Pitch Decision-Making With MLB's Statcast Data

By **Max Wittenberg**

Introduction

The Oakland Athletics baseball team in 2002 used data analysis and quantitative modeling to identify undervalued players and create a competitive lineup on a limited budget. The book "Moneyball," written by Michael Lewis, highlighted the A's '02 season and gave an inside glimpse into how unique the team's strategic data modeling was for its time. Fast-forward 20 years — the use of data science and quantitative modeling is now a common practice among all sports franchises and plays a critical role in scouting, roster construction, game-day operations and season planning.

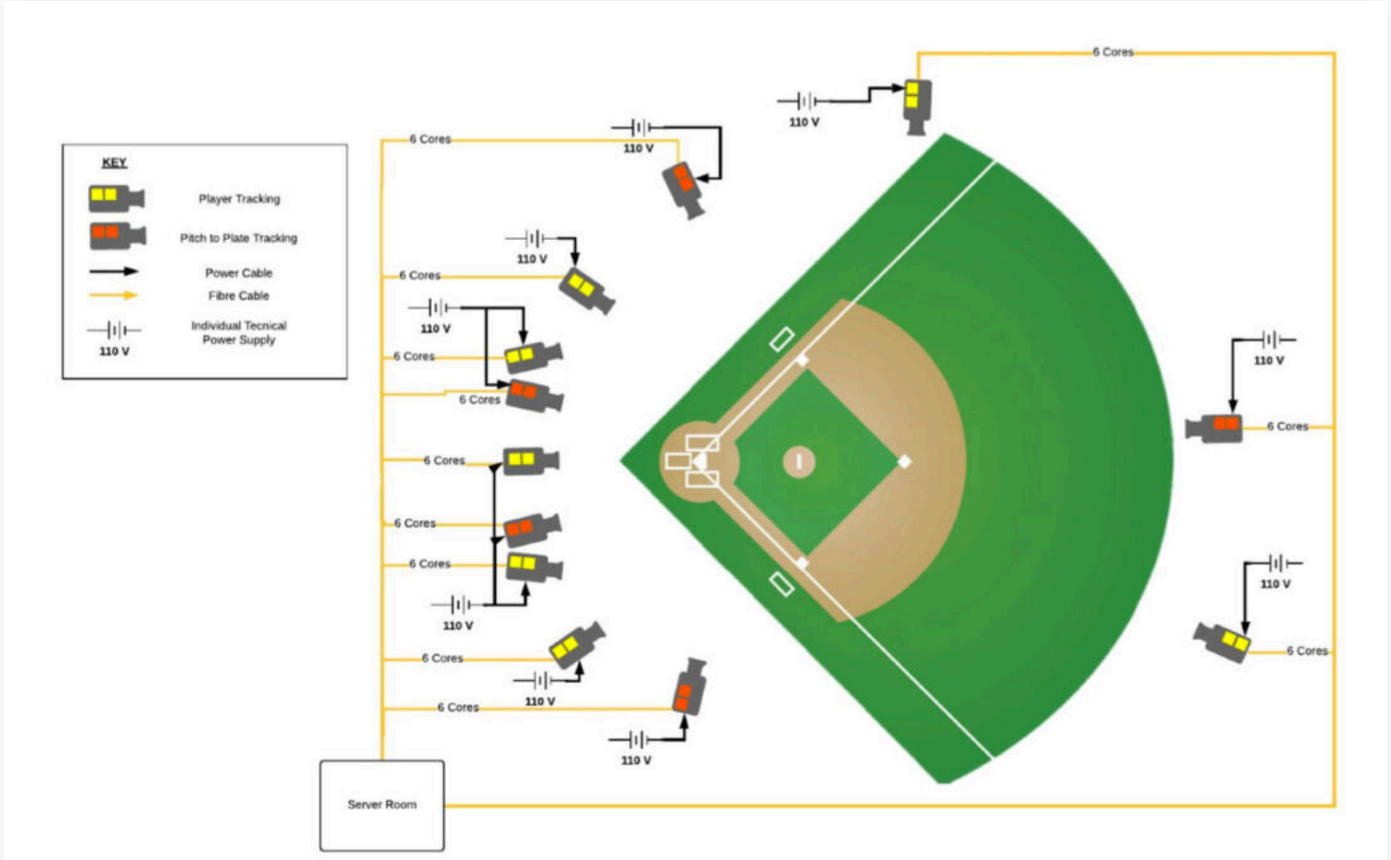


Figure 1: Position and scope of Hawkeye cameras at a baseball stadium

In 2015, Major League Baseball (MLB) introduced Statcast, a set of cameras and radar systems installed in all 30 MLB stadiums. Statcast generates up to seven terabytes of data during a game, capturing every imaginable data point and metric related to pitching, hitting, running and fielding, which the system collects and organizes for consumption. This explosion of data has created opportunities to analyze the game in real time, and with the application of machine learning, teams are now able to make decisions that influence the outcome of the game, pitch by pitch. It's been 20 seasons since the A's first introduced the use of data modeling to baseball. Here's an inside look at how professional baseball teams use technologies like Databricks to create the modern-day "Moneyball" and gain competitive advantages that data teams provide to coaches and players on the field.

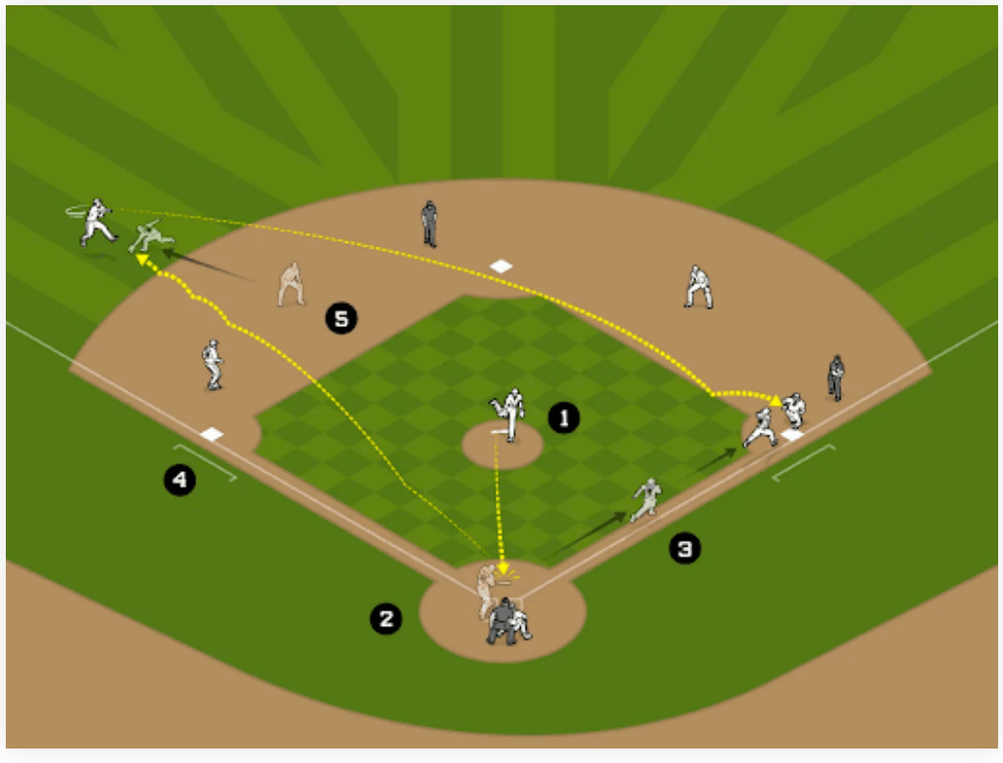


Figure 2: Numbers represent events during a play captured by Statcast

pitch_type	game_date	release_speed	release_pos_x	release_pos_z	player_name	batter	pitcher	events	description
SI	2020-09-18T00:00:00.000+0000	91	1.59	5.02	Sherriff, Ryan	600524	595411	field_out	hit_into_play
SI	2020-09-18T00:00:00.000+0000	90.8	1.57	5	Sherriff, Ryan	600524	595411	NaN	foul
SI	2020-09-18T00:00:00.000+0000	91.2	1.8	4.95	Sherriff, Ryan	600524	595411	NaN	ball
SI	2020-09-18T00:00:00.000+0000	91.4	1.83	4.81	Sherriff, Ryan	600524	595411	NaN	ball
SI	2020-09-18T00:00:00.000+0000	91	1.69	4.93	Sherriff, Ryan	600524	595411	NaN	called_strike
SI	2020-09-18T00:00:00.000+0000	90.5	1.74	4.84	Sherriff, Ryan	669720	595411	field_out	hit_into_play
SI	2020-09-18T00:00:00.000+0000	91.8	1.7	4.96	Sherriff, Ryan	669720	595411	NaN	called_strike
SI	2020-09-18T00:00:00.000+0000	89.7	1.6	4.95	Sherriff, Ryan	578428	595411	field_out	hit_into_play
SI	2020-09-18T00:00:00.000+0000	89.8	1.61	5.01	Sherriff, Ryan	578428	595411	NaN	called_strike
FF	2020-09-18T00:00:00.000+0000	95	2.9	5.38	Scott, Tanner	664040	656945	field_out	hit_into_play

Figure 3: Sample of data collected by Statcast

Background

Data teams need to be faster than ever to provide analytics to coaches and players so they can make decisions as the game unfolds. The decisions made from real-time analytics can dramatically change the outcome of a game and a team's season. One of the more memorable examples of this was in game six of the 2020 World Series. The Tampa Bay Rays were leading the Los Angeles Dodgers 1-0 in the sixth inning when Rays pitcher Blake Snell was pulled from the mound while pitching arguably one of the best games of his career, a decision head coach Kevin Cash said was made with the insights from their data analytics. The Rays went on to lose the game and World Series. Hindsight is always 20-20, but it goes to show how impactful data has become to the game. Coaching staff task their data teams with assisting them in making critical decisions — for example, should a pitcher throw another inning or make a substitution to avoid a potential injury? Does a player have a greater probability of success stealing from first to second base, or from second to third?

I have had the opportunity to work with many MLB franchises and discuss what their priorities and challenges are related to data analytics. Typically, I hear three recurring themes their data teams are focused on that have the most value in helping set their team up for success on the field:

1. **Speed:** Since every MLB team has access to the Statcast data during a game, one way to create a competitive advantage is to ingest and process the data faster than your opponent. The average length of time between pitches is 23 seconds, and this window of time represents a benchmark from which Statcast data can be ingested and processed for coaches to use to make decisions that can impact the outcome of the game.
2. **Real-Time Analytics:** Another competitive advantage for teams is the creation of insights from their machine learning models in real time. An example of this is knowing when to substitute out a pitcher from fatigue, where a model interprets pitcher movement and data points created from the pitch itself and is able to forecast deterioration of performance pitch by pitch.
3. **Ease of Use:** Analytics teams run into problems ingesting the volumes of data Statcast produces when running data pipelines on their local computers. This gets even more complicated when trying to scale their pipelines to capture minor league data and integrate with other technologies. Teams want a collaborative, scalable analytics platform that automates data ingestion with performance, creating the ability to impact in-game decision-making.

Baseball teams using Databricks have developed solutions for these priorities and several others. They have shaped what the modern-day version of "Moneyball" looks like. What follows is their successful framework explained in an easy-to-understand way.

Getting the data

When a pitcher throws a baseball, Hawkeye cameras collect the data and save it to an application that teams are able to access using an application programming interface (API) owned by MLB. You can think of an API as an intermediate connection between two computers to exchange information. The way this works is: a user sends a request to an API, the API confirms that the user has permission to access the data and then sends back the requested data for the user to consume. To use a restaurant as an analogy – a customer tells a waiter what they want to eat, the waiter informs the kitchen what the customer wants to eat, the waiter serves the food to the customer. The waiter in this scenario is the API.

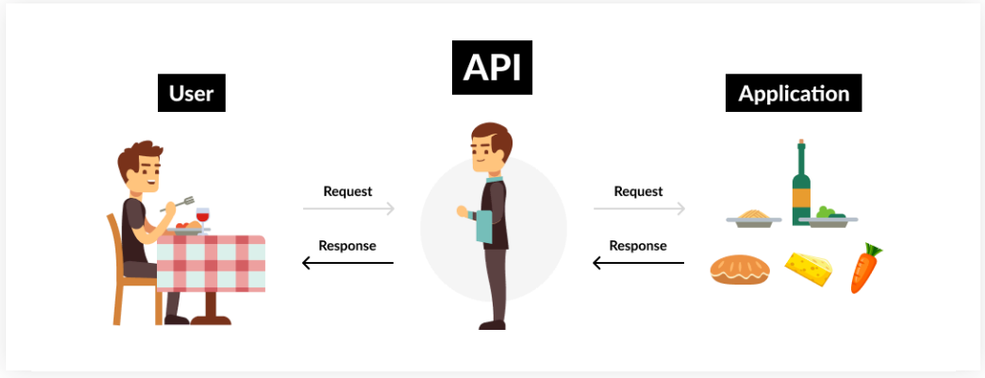


Figure 4: Example of how an API works, using a restaurant analogy

This simple method of retrieving data is called a "batch" style of data collection and processing, where data is gathered and processed once. As noted earlier, however, data is typically available through the API every 23 seconds (the average time between pitches). This means data teams need to make continuous requests to the API in a method known as "streaming," where data is continuously collected and processed. Just as a waiter can quickly become overworked fulfilling customers' needs, making continuous API requests for data creates some challenges in data pipelines. With the assistance from these data teams, however, we have created code to accommodate continuously collecting Statcast data during a game. You can see an example of the code using a test API below.

```
from pathlib import Path
import json

class sports_api:
    def __init__(self, endpoint, api_key):
        self.endpoint = endpoint
        self.api_key = api_key
        self.connection = self.endpoint + self.api_key

    def fetch_payload(self, request_1, request_2, adls_path):
        url = f"{self.connection}&series_id={request_1}{request_2}-
99.M"
        r = requests.get(url)
        json_data = r.json()
        now = time.strftime("%Y%m%d-%H%M%S")
        file_name = f"json_data_out_{now}"
        file_path = Path("dbfs:/") / Path(adls_path) / Path(file_name)
        dbutils.fs.put(str(file_path), json.dumps(json_data), True)
        return str(file_path)
```

Figure 5: Interacting with an API to retrieve and save data

This code decouples the steps of getting data from the API and transforming it into usable information, which in the past, we have seen, can cause latency in data pipelines. Using this code, the Statcast data is saved as a file to cloud storage automatically and efficiently. The next step is to ingest it for processing.

Automatically load data with Auto Loader

As pitch and play data is continuously saved to cloud storage, it can be ingested automatically using a Databricks feature called Auto Loader. Auto Loader scans files in the location they are saved in cloud storage and loads the data into Databricks where data teams begin to transform it for their analytics. Auto Loader is easy to use and incredibly reliable when scaling to ingest larger volumes of data in batch and streaming scenarios. In other words, Auto Loader works just as well for small and large data sizes in batch and streaming scenarios. The Python code below shows how to use Auto Loader for streaming data.

```
df = spark.readStream.format("cloudFiles") \
    .option(,) \
    .schema() \
    .load()

df.writeStream.format("delta") \
    .option("checkpointLocation", ) \
    .trigger() \
    .start()
```

Figure 6: Setup of Auto Loader to stream data

One challenge in this process is working with the file format in which the Statcast is saved, a format called JSON. We are typically privileged to work with data that is already in a structured format, such as the CSV file type, where data is organized in columns and rows. The JSON format organizes data into arrays and despite its wide use and adoption, I still find it difficult to work with, especially in large sizes. Here's a comparison of data saved in a CSV format and a JSON format.

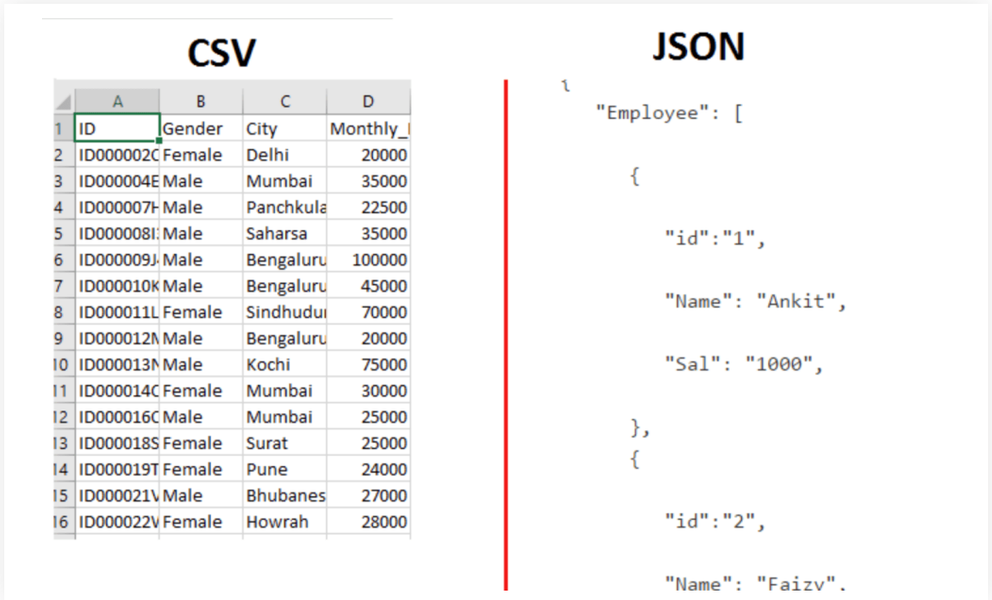


Figure 7: Comparison of CSV and JSON formats

It should be obvious which of these two formats data teams prefer to work with. The goal then is to load Statcast data in the JSON format and transform it into the friendlier CSV format. To do this, we can use the semi-structured data support available in Databricks, where basic syntax allows us to extract and transform the nested data you see in the JSON format to the structured CSV style format. Combining the functionality of Auto Loader and the simplicity of semi-structured data support creates a powerful data ingestion method that makes the transformation of JSON data easy.

Using Databricks' semi-structured data support with Auto Loader

```
spark.readStream.format("cloudFiles") \
    .option("cloudFiles.format", "json") \
    .option("cloudFiles.schemaLocation", "") \
    .load("") \
    .selectExpr(
    "*",
    "tags:page.name", # extracts {"tags":{"page":{"name":...}}}
    "tags:page.id::int", # extracts {"tags":{"page":{"id":...}}} and
casts to int
    "tags:eventType" # extracts {"tags":{"eventType":...}}
    )
```

As the data is loaded in, we save it to a Delta table to start working with it further. Delta Lake is an open format storage layer that brings reliability, security and performance to a data lake for both streaming and batch processing and is the foundation of a cost-effective, highly scalable data platform. Semi-structured support with Delta allows you to retain some of the nested data if needed. The syntax allows flexibility to maintain nested data objects as a column within a Delta table without the need to flatten out all of the JSON data. Baseball analytics teams use Delta to version Statcast data and enforce specific needs to run their analytics on while organizing it in a friendly structured format.

Auto Loader writing data to a Delta table as a stream

```
# Define the schema and the input, checkpoint, and output paths.
read_schema = ("id int, " +
    "firstName string, " +
    "middleName string, " +
    "lastName string, " +
    "gender string, " +
    "birthDate timestamp, " +
    "ssn string, " +
    "salary int")
json_read_path = '/FileStore/streaming-uploads/people-10m'
checkpoint_path = '/mnt/delta/people-10m/checkpoints'
save_path = '/mnt/delta/people-10m'

people_stream = (spark \
    .readStream \
    .schema(read_schema) \
    .option('maxFilesPerTrigger', 1) \
    .option('multiline', True) \
    .json(json_read_path))

people_stream.writeStream \
    .format('delta') \
    .outputMode('append') \
    .option('checkpointLocation', checkpoint_path) \
    .start(save_path)
```

With Auto Loader continuously streaming in data after each pitch, semi-structured data support transforming it into a consumable format, and Delta Lake organizing it for use, data teams are now ready to build analytics that gives their team the competitive edge on the field.

Machine learning for insights

Recall the Rays pulling Blake Snell from the mound during the World Series — that decision came from insights coaches saw in their predictive models. Statistical analysis of Snell's historical Statcast data provided by Billy Heylen of sportingnews.com indicated Snell had not pitched more than six innings since July 2019, had a lower probability of striking out a batter when facing them for the third time in a game, and was being relieved by teammate Nick Anderson, whose own pitch data suggests was one the strongest closers in MLB, with a 0.55 earned run average (ERA) and 0.49 walks and hits per innings pitched (WHIP) during the 19 regular-season games he pitched in 2020. Predictive models analyze data like this in real time and provide supporting evidence and recommendations coaches use to make critical decisions.

Machine learning models are relatively easy to build and use, but data teams often struggle to implement them into streaming use cases. Add in the complexity of how models are managed and stored and machine learning can quickly become out of reach. Fortunately, data teams use MLflow to manage their machine learning models and implement them into their data pipelines. MLflow is an open source platform for managing the end-to-end machine learning lifecycle and includes support for tracking predictive results, a model registry for centralizing models that are in use and others in development, and a serving capability for using models in data pipelines.

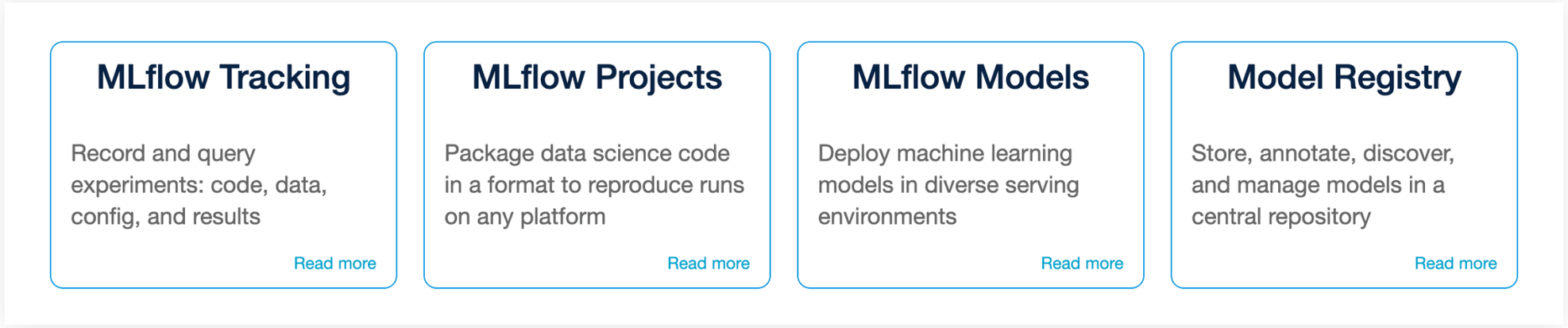


Figure 8: MLflow overview

To implement machine learning algorithms and models to real-time use cases, data teams use the model registry where a model is able to read data sitting in a Delta table and create predictions that are then used during the game. Here's an example of how to use a machine learning model while data is automatically loaded with Auto Loader:

Getting a machine learning model from the registry and using it with Auto Loader

```
#get model from the model registry
model = mlflow.spark.load_model(
    model_uri=f"models:/{model_name}/{'Production'}")

#read data from bronze table as a stream
events = spark.readStream \
    .format("delta") \
    #.option("cloudFiles.maxFilesPerTrigger", 1)\
    .schema(schema) \
    .table("baseball_stream_bronze")

#pass stream through model
model_output = model.transform(events)

#write stream to silver delta table
events.writeStream \
    .format('delta') \
    .outputMode("append") \
    .option('checkpointLocation', "/tmp/baseball/") \
    .table("default.baseball_stream_silver")
```

The outputs a machine learning model creates can then be displayed in a data visualization or dashboard and used as printouts or shared on a tablet during a game. MLB franchises working on Databricks are developing fascinating use cases that are being used during games throughout the season. Predictive models are proprietary to the individual teams, but here's an actual use case running on Databricks that demonstrates the power of real-time analytics in baseball.

Bringing it all together with spin ratios and sticky stuff

MLB introduced a new rule for the 2021 season meant to discourage pitcher's use of "sticky stuff," a substance hidden in mitts, belts or hats that when applied to a baseball can dramatically increase the spin ratio of a pitch, making it difficult for batters to hit. The rule suspends for 10 games pitchers discovered using sticky stuff. Coaches on opposing teams have the ability to request an umpire check for the substance if they suspect a pitcher to be using it during a game. Spin ratio is a data point that is captured by Hawkeye cameras, and with real-time analytics and machine learning, teams are now able to make justified requests to umpires with the hopes of catching a pitcher using the material.

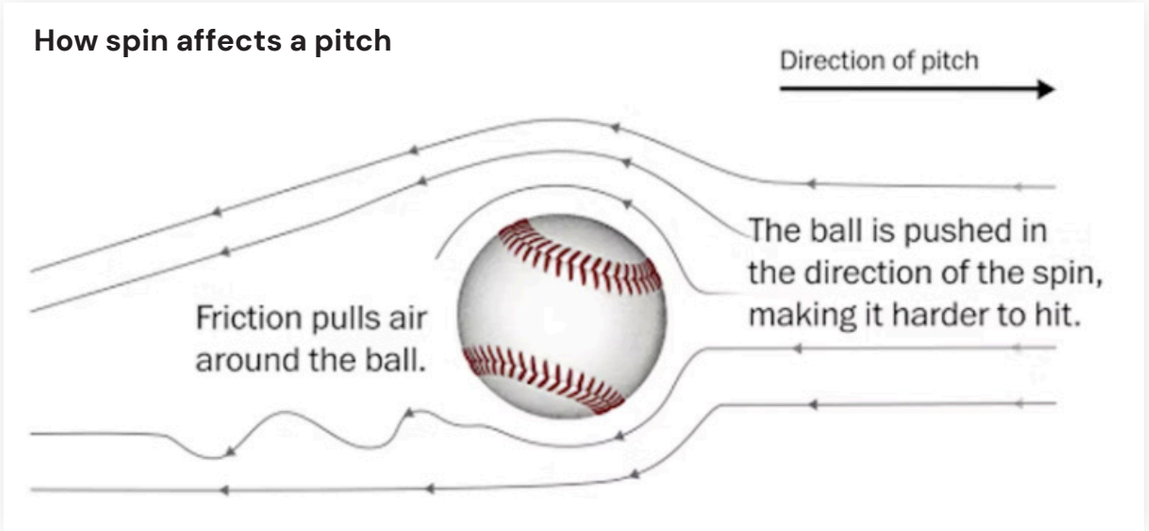


Figure 9: Illustration of how spin affects a pitch

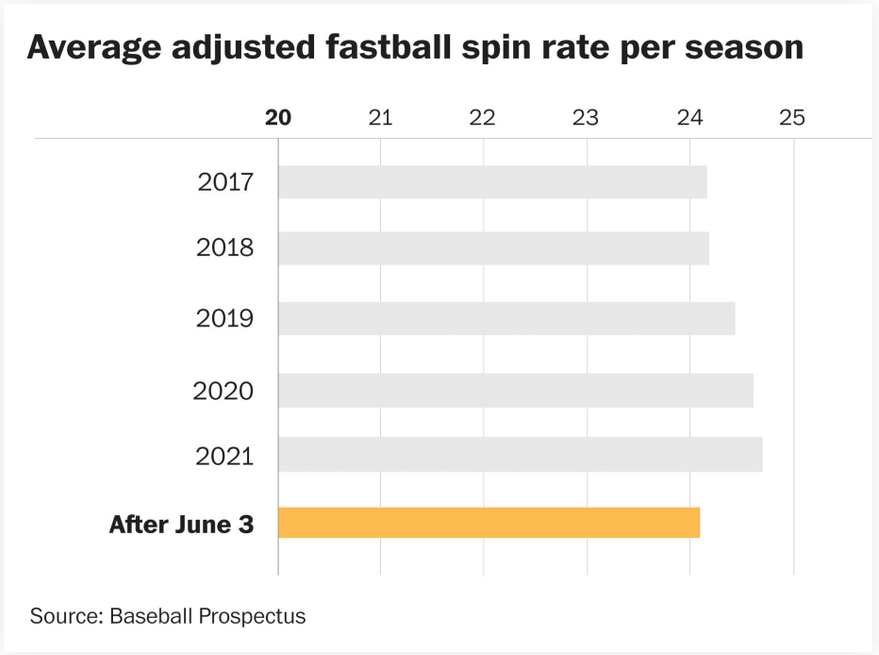


Figure 10: Trending spin rate of fastballs per season and after rule introduction on June 3, 2021

Following the same framework outlined above, we ingest Statcast data pitch by pitch and have a dashboard that tracks the spin ratio of the ball for all pitchers during all MLB games. Using machine learning models, predictions are sent to the dashboard that flag outliers against historical data and the pitcher's performance in the active game, which can alert coaches when they fall outside of ranges anticipated by the model. With Auto Loader, Delta Lake and MLflow, all data ingestion and analytics happen in real time.

Technologies like Statcast and Databricks have brought real-time analytics to sports and changed the paradigm of what it means to be a data-driven team. As data volumes continue to grow, having the right architecture in place to capture real-time insights will be critical to staying one step ahead of the competition. Real-time architectures will be increasingly important as teams acquire and develop players, plan for the season and develop an analytically enhanced approach to their franchise. Ask about our Solution Accelerator with Databricks partner Lovelytics, which provides sports teams with all the resources they need to quickly create use cases like the ones described in this blog.

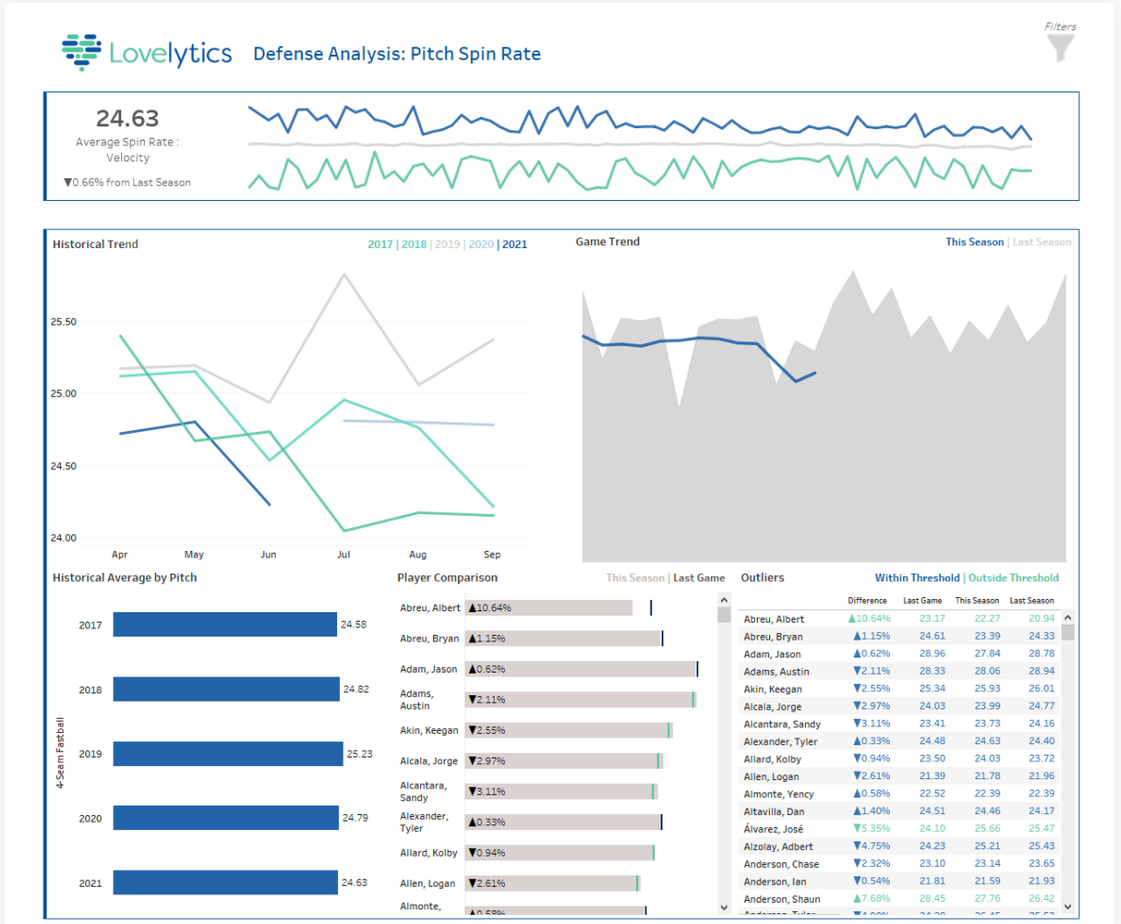


Figure 11: Dashboard for “sticky stuff” detection in real time

CHAPTER 3:

Improving On-Shelf Availability for Items With AI Out-of-Stock Modeling

This post was written in collaboration with Databricks partner Tredence. We thank Rich Williams, Vice President Data Engineering, and Morgan Seybert, Chief Business Officer, of Tredence for their contributions.

By **Rich Williams, Morgan Seybert, Rob Saker** and **Bryan Smith**

Introduction

Retailers are missing out on nearly $1 trillion in global sales because they don't have on hand what customers want to buy in their stores. Adding to the challenge, a study of 600 households and several retailers by research firm IHL Group details that shoppers encounter out-of-stocks (OOS) as often as one in three shopping trips, according to the report. And a study by IRI found that 20% of all out-of-stocks remain unresolved for more than 3 days.

Overall, studies show that the average OOS rate is about 8%. That means that one out of 13 products is not purchasable at the exact moment the customer wants to get it in the store. OOS is one of the biggest problems in retail, but thankfully it can be solved with real-time data and analytics.

In this write-up, we showcase the new Tredence-Databricks combined On-Shelf Availability Solution Accelerator. The accelerator is a robust quick-start guide that is the foundation for a full out-of-stock or supply chain solution. We outline how to approach out-of-stocks with the Databricks Lakehouse to solve for on-shelf availability in real time.

And the impact of solving this problem? A 2% improvement in on-shelf availability is worth 1% in increased sales for retailers.

Growth in e-commerce makes item availability more important

The significance of this problem has been amplified by the availability of e-commerce for delivery and curbside pickup orders. While customers that face an out-of-stock at the store level may just not purchase that item, they are likely to purchase other items in the store. Buying online means that they may just switch to a different retailer.

The impact is not just limited to a bottom line loss in revenue. Research from NielsenIQ shows that 30% of shoppers will visit new stores when they can't find the product they are looking for, leading to a loss in long-term loyalty. Members of e-commerce membership programs are most likely to switch retailers in the event of an out-of-stock. IHL estimates that "upwards of 24% of Amazon's current retail revenue comes from customers who first tried to buy the product in-store."

Retailers have responded to this with a variety of tactics including over-ordering of items, which increases carrying costs and lowers margins when they are forced to sell excess inventory at a discount. In some instances, retailers and distributors will rush order products or use intra-delivery "hot shots" for additional deliveries, which come at an additional cost. Some retailers have invested in robotics, but many pull out of their pilots citing costs. And other retailers are experimenting with computer vision, although these approaches merely notify them when an item is unavailable and don't predict item availability.

It's not just retailers that are impacted by OOS. Retailers, consumer goods companies, distributors, brokers and other firms each invest in third-party audits, which typically involve employees visiting stores to identify gaps on the shelf. On any given day, tens of thousands of individuals are visiting stores to validate item availability. Is this really the best use of time and resources?

Why hasn't technology solved out-of-stocks yet?

Out-of-stock issues have been around for decades, so why hasn't the retail industry been able to solve an issue of this magnitude that impacts shoppers, retailers and brands alike? The seemingly simple solution is to require employees to manually count the items on hand. But with potentially hundreds of thousands of individual SKUs distributed across a large format retail location that may be servicing customers nearly 24 hours a day, this simply isn't a realistic task to perform on a regular basis.

Individual stores do perform inventory counts periodically and then rely on point-of-sale (POS) and inventory management software to track changes that drive unit counts up and down. But with so much activity within a store location, some of the day-to-day recordkeeping falls through the cracks, not to mention the impact of shrinkage, which can be hard to detect, on in-store supplies.

So the industry falls back on modeling. But given fundamental problems in data accuracy, these approaches can drive a combination of false positives and false negatives that make model predictions difficult to employ. Time sensitivities further exacerbate the problem, as the large volume of data that often must be crunched in order to arrive at model predictions must be handled fast enough for the results to be actionable. The problem of building a reliable system for stockout prediction and alerting is not as straightforward as it might appear.

Introducing the On-Shelf Availability Solution Accelerator

Our partners at Tredence approached us with the idea of publishing a Solution Accelerator that they've created as the core of a broader Supply Chain Control Tower offering. Tredence works with the largest retailers on the planet and understands the nuances of modeling OOS and knew that Databricks' processing and their advanced data science capabilities were a winning combination.

While the OSA solution focuses on driving sales through improved stock availability on the shelves, the broader Retail Supply Chain Control Tower solves for multiple adjacent merchandising problems – inventory design for the stores, efficient store replenishments, design of store network for omnichannel operations, etc. Knowing how big a problem this is in retail, we immediately took them up on their offer.

The first step in addressing OSA challenges is to examine their occurrence in the historical data. Past occurrences point to systemic issues with suppliers and internal processes, which will continue to cause problems if not addressed.

To support this analysis, Tredence made available a set of historical inventory and sales data. These data sets were simulated, given the obvious sensitivities any retailer would have around this information, but were created in a manner that frequently observed OSA challenges manifested in the data. These challenges were:

1. **Phantom inventory**
2. **Safety stock violations**
3. **Zero-sales events**
4. **On-shelf availability**

Phantom inventory

In a phantom inventory scenario, the units reported to be on hand do not align with units expected based on reported sales and replenishment.

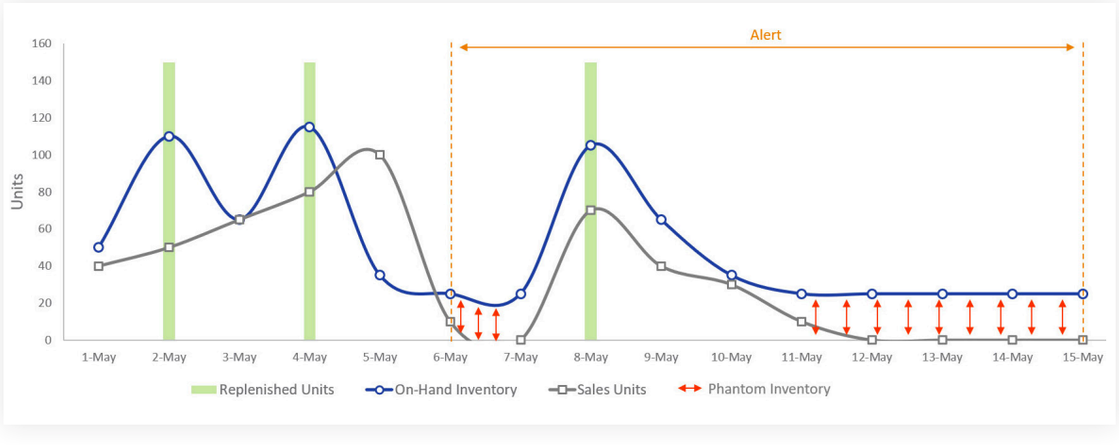


Figure 1: The misalignment of reported inventory, with inventory expected based on sales and replenishment, creating phantom inventory

Poor tracking of replenishment units, unreported or undetected shrinkage, and out-of-band processes coupled with infrequent and sometimes inaccurate inventory counts create a situation where retailers believe they have more units on hand than they actually do. If large enough, this phantom inventory may delay or even prevent the ordering of replenishment units, leading to an out-of-stock scenario.

Safety stock violations

Most organizations establish a threshold for a given product's inventory, below which replenishment orders are triggered. If set too low, inadequate lead times or even minor disruptions to the supply chain may lead to an out-of-stock scenario while new units are moving through the replenishment pipeline.

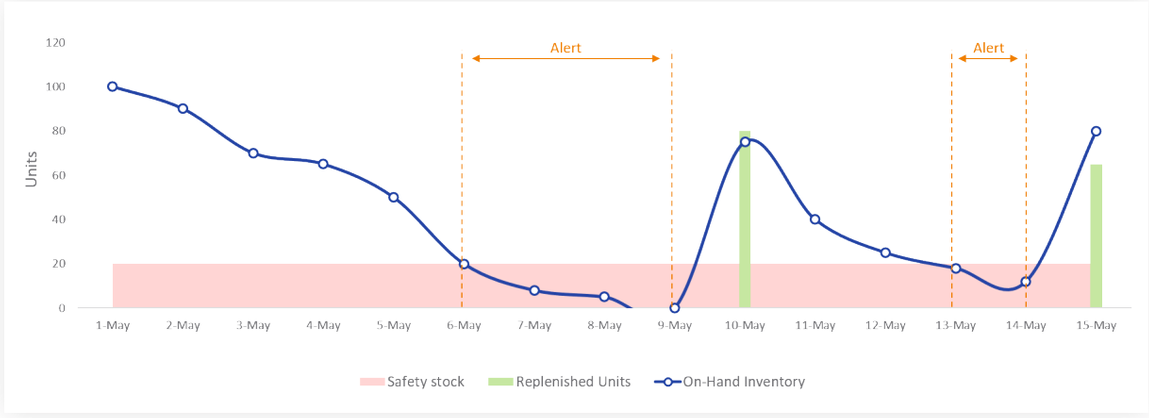


Figure 2: Safety stock levels not providing adequate lead time to prevent out-of-stock issues

The flip side of this is that if set too high, retailers risk overstocking products that may expire, risk damage or theft, or otherwise consume space and capital that may be better employed in other areas. Finding the right safety stock level for a product in a specific location is a critical task for effective inventory management.

Zero-sales events

Phantom inventory and safety stock violations are the two most common causes of out-of-stocks. Regardless of the cause, out-of-stock events manifest themselves in periods when no units of a product are sold.

Not every occurrence of a zero-sales event reflects an out-of-stock concern. Some products don't sell every day, and for some slow-moving products, multiple days may go by within which zero units are sold while the product remains adequately stocked.

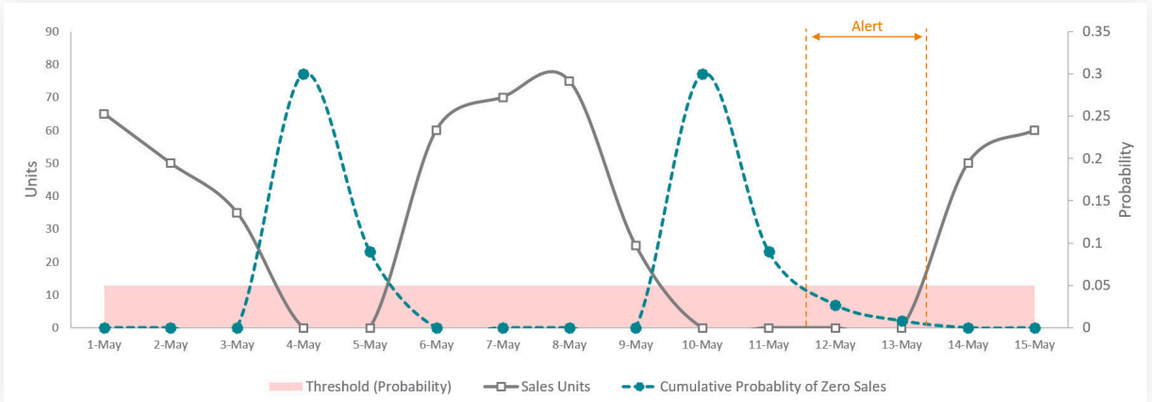


Figure 3: Examining the cumulative probability of consecutive zero-sales events to identify potential out-of-stock issues

The trick for scrutinizing zero-sales events at the item level is to understand the probability of which at least one unit of a product sells on a given day and to then set a cumulative probability threshold for consecutive days reflecting zero-sales. When the cumulative probability of back-to-back zero-sales events exceeds the threshold, it's time for the inventory of that product to be examined.

On-shelf availability

While understanding scenarios in which items are not in stock is critical, it's equally important to recognize when products are technically available for sale but underperforming because of non-optimal inventory management practices. These merchandising problems may be due to poor placement of displays within the store, the stocking of products deep within a shelf, the slow transfer of product from the backroom to shelves, or a myriad of other scenarios in which inventory is adequate to meet demand but customers cannot easily view or access it.

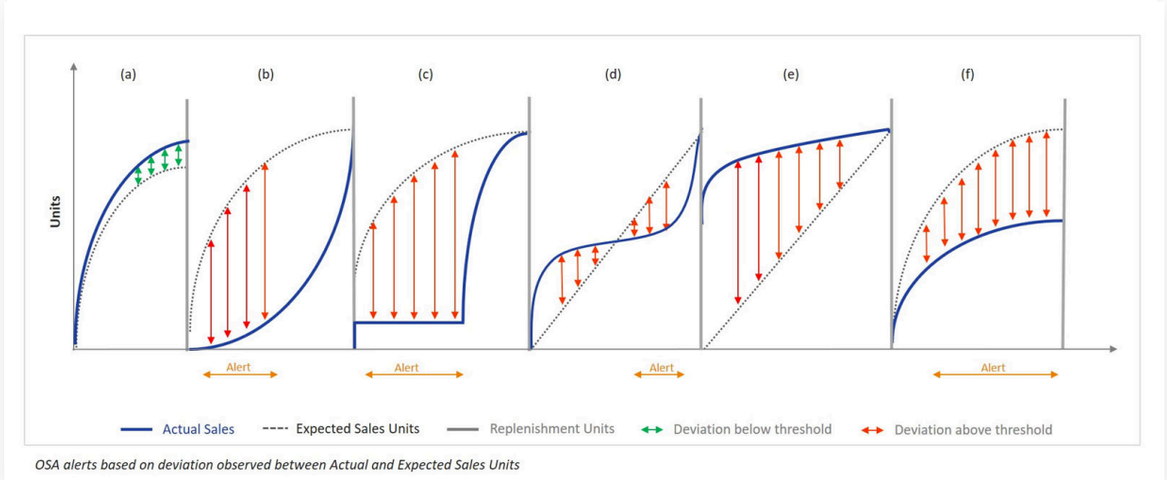


Figure 4: Depressed sales due to poor product placement leading to an on-shelf availability problem

To detect these kinds of problems, it is helpful to compare actual sales to those forecasted for the period. While not every missed sales goal indicates an on-shelf availability problem, a sustained miss might signal a problem that requires further attention.

How we approach out-of-stocks with the Databricks Lakehouse Platform

The evaluation of phantom inventories, safety stock violations, zero-sales events and on-shelf availability problems requires a platform capable of performing a wide range of tasks. Inventory and sales data must be aggregated and reconciled at a per-period level. Complex logic must be applied across these data to examine aggregate and series patterns. Forecasts may need to be generated for a wide range of products across numerous locations. And the results of all this work must be made accessible to the business analysts responsible for scrutinizing the findings before soliciting action from those in the field.

Databricks provides a single platform capable of all this work. The elastic scalability of the platform ensures that the processing of large volumes of data can be performed in an efficient and timely manner. The flexibility of its development environment allows data engineers to pivot between common languages, such as SQL and Python, to perform data analysis in a variety of modes.

Pre-integrated libraries provide support for classic time series forecasting algorithms and techniques, and easy programmatic installations of alternative libraries such as Facebook Prophet allow data scientists to deliver the right forecast for the business's needs. Scalable patterns ensure data science tasks are also tackled in an efficient and timely manner with little deviation from the standard approaches data scientists typically employ.

And the SQL Analytics interface, as well as robust integrations with Tableau and Power BI, allows analysts to consume the results of the data scientists' and data engineers' work without having to first port the data to alternative platforms.

Getting started

Be sure to check out and download the notebooks for out-of-stock modeling. As with any of our Solution Accelerators, these are a foundation for a full solution. If you would like help with implementing a full out-of-stock or supply chain solution, go visit our friends at Tredence.

To see these features in action, please check out the following notebooks demonstrating how Tredence tackled out-of-stocks on the Databricks platform:

> OSA 1: Data Preparation →
> OSA 2: Out-of-Stocks →
> OSA 3: On-Shelf Availability →

CHAPTER 4:

Using Dynamic Time Warping and MLflow to Detect Sales Trends

Part 1 of our Using Dynamic Time Warping and MLflow to Detect Sales Trends series

By **Ricardo Portilla**, **Brenner Heintz** and **Denny Lee**

Try this notebook in Databricks →

Introduction

The phrase "dynamic time warping," at first read, might evoke images of Marty McFly driving his DeLorean at 88 MPH in the "Back to the Future" series. Alas, dynamic time warping does not involve time travel; instead, it's a technique used to dynamically compare time series data when the time indices between comparison data points do not sync up perfectly.

As we'll explore below, one of the most salient uses of dynamic time warping is in speech recognition — determining whether one phrase matches another, even if the phrase is spoken faster or slower than its comparison. You can imagine that this comes in handy to identify the "wake words" used to activate your Google Home or Amazon Alexa device — even if your speech is slow because you haven't yet had your daily cup(s) of coffee.

Dynamic time warping is a useful, powerful technique that can be applied across many different domains. Once you understand the concept of dynamic time warping, it's easy to see examples of its applications in daily life, and its exciting future applications. Consider the following uses:

- **Financial markets:** comparing stock trading data over similar time frames, even if they do not match up perfectly. For example, comparing monthly trading data for February (28 days) and March (31 days).
- **Wearable fitness trackers:** more accurately calculating a walker's speed and the number of steps, even if their speed varied over time
- **Route calculation:** calculating more accurate information about a driver's ETA, if we know something about their driving habits (for example, they drive quickly on straightaways but take more time than average to make left turns)

Data scientists, data analysts and anyone working with time series data should become familiar with this technique, given that perfectly aligned time series comparison data can be as rare to see in the wild as perfectly "tidy" data.

In this blog series, we will explore:

- The basic principles of dynamic time warping
- Running dynamic time warping on sample audio data
- Running dynamic time warping on sample sales data using MLflow

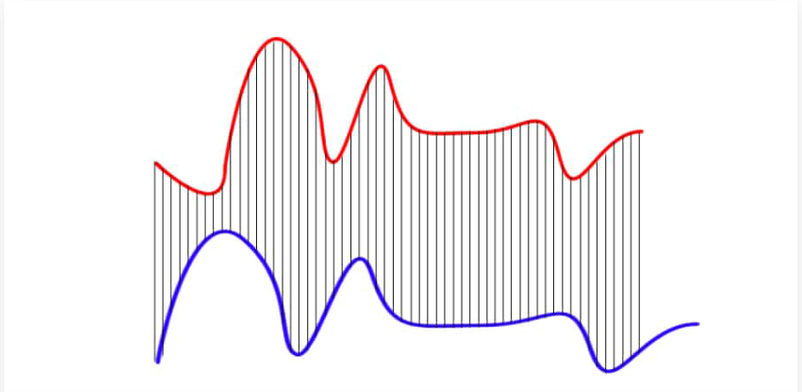
Dynamic time warping

The objective of time series comparison methods is to produce a *distance metric* between two input time series. The similarity or dissimilarity of two time series is typically calculated by converting the data into vectors and calculating the Euclidean distance between those points in vector space.

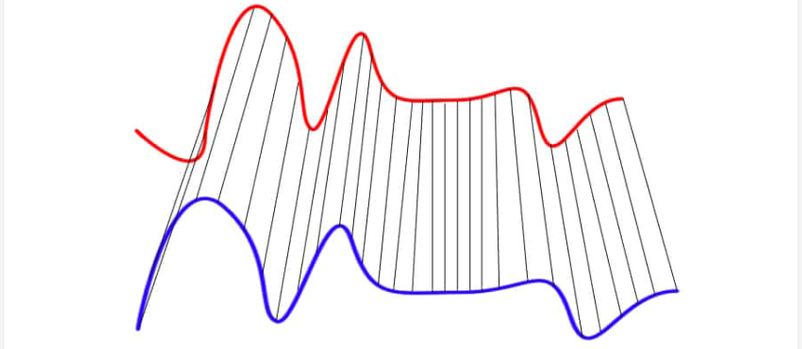
Dynamic time warping is a seminal time series comparison technique that has been used for speech and word recognition since the 1970s with sound waves as the source; an often cited paper is "Dynamic time warping for isolated word recognition based on ordered graph searching techniques."

Background

This technique can be used not only for pattern matching, but also anomaly detection (e.g., overlap time series between two disjoint time periods to understand if the shape has changed significantly, or to examine outliers). For example, when looking at the red and blue lines in the following graph, note the traditional time series matching (i.e., Euclidean matching) is extremely restrictive. On the other hand, dynamic time warping allows the two curves to match up evenly even though the X-axes (i.e., time) are not necessarily in sync. Another way to think of this is as a robust dissimilarity score where a lower number means the series is more similar.



EUCLIDEAN MATCHING



DYNAMIC TIME WARP MATCHING

Source: Wikimedia Commons
File: Euclidean_vs_DTW.jpg

Two time series (the base time series and new time series) are considered similar when it is possible to map with function f(x) according to the following rules so as to match the magnitudes using an optimal (warping) path.

$$f(x_i) \text{ maps to } f(x_j) \text{ when } i <= j$$

$$f(x_i) \text{ maps to } f(x_j) \text{ only when } (j - i) \text{ is within fixed range}$$

Sound pattern matching

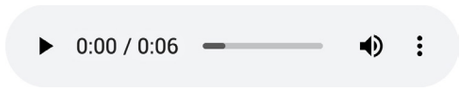
Traditionally, dynamic time warping is applied to audio clips to determine the similarity of those clips. For our example, we will use four different audio clips based on two different quotes from a TV show called The Expanse. There are four audio clips (you can listen to them below, but this is not necessary) — three of them (clips 1, 2 and 4) are based on the quote

"Doors and corners, kid. That's where they get you."

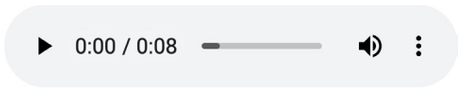
And in one clip (clip 3) is the quote

"You walk into a room too fast, the room eats you."

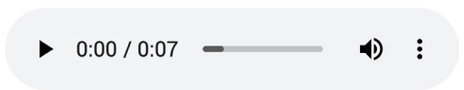
Clip 1 | Doors and corners, kid. That's where they get you. [v1]



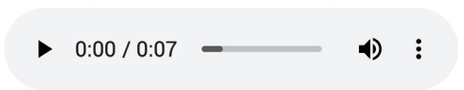
Clip 2 | Doors and corners, kid. That's where they get you. [v2]



Clip 3 | You walk into a room too fast, the room eats you.



Clip 4 | Doors and corners, kid. That's where they get you. [v3]

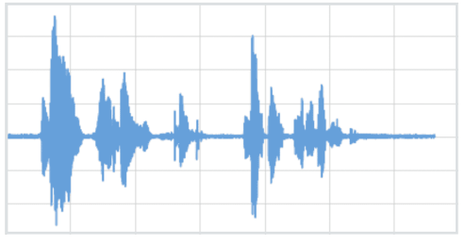


Quotes are from "The Expanse"

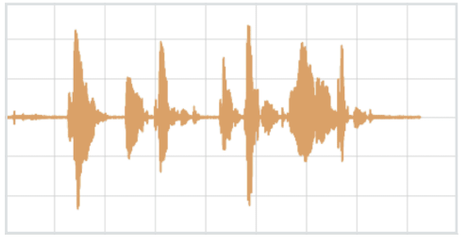
Below are visualizations using `matplotlib` of the four audio clips:

- **Clip 1:** This is our base time series based on the quote "Doors and corners, kid. That's where they get you."
- **Clip 2:** This is a new time series [v2] based on clip 1 where the intonation and speech pattern are extremely exaggerated
- **Clip 3:** This is another time series that's based on the quote "You walk into a room too fast, the room eats you." with the same intonation and speed as clip 1
- **Clip 4:** This is a new time series [v3] based on clip 1 where the intonation and speech pattern is similar to clip 1

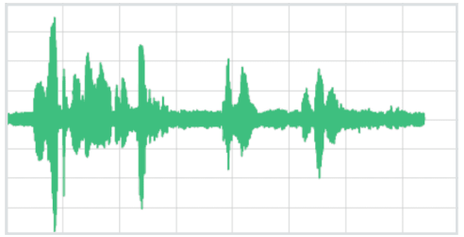
Clip 1 | Doors and corners, kid. That's where they get you. [v1]



Clip 2 | Doors and corners, kid. That's where they get you. [v2]



Clip 3 | You walk into a room too fast, the room eats you.



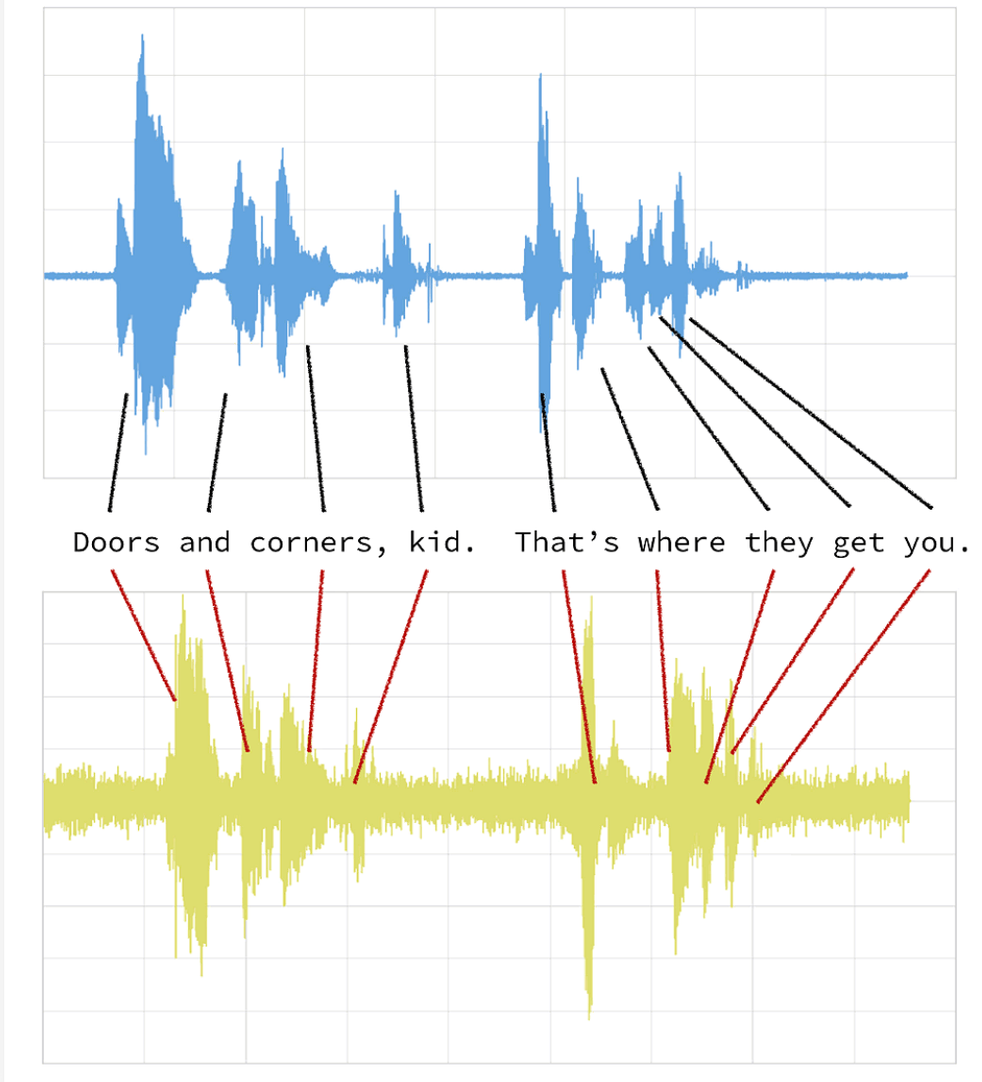
Clip 4 | Doors and corners, kid. That's where they get you. [v3]

The code to read these audio clips and visualize them using Matplotlib can be summarized in the following code snippet.

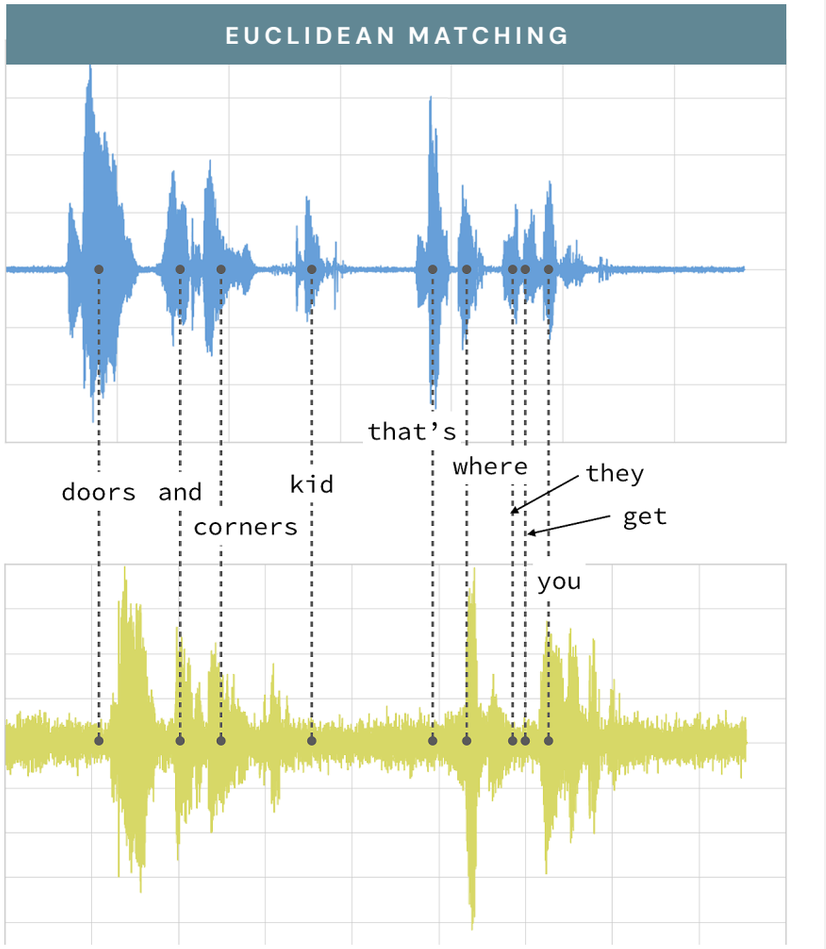
```
from scipy.io import wavfile
from matplotlib import pyplot as plt
from matplotlib.pyplot import figure

# Read stored audio files for comparison
fs, data = wavfile.read("/dbfs/folder/clip1.wav")

# Set plot style
plt.style.use('seaborn-whitegrid')

# Create subplots
ax = plt.subplot(2, 2, 1)
ax.plot(data1, color='#67A0DA')
...

# Display created figure
fig=plt.show()
display(fig)
```

The full code base can be found in the notebook Dynamic Time Warping Background.

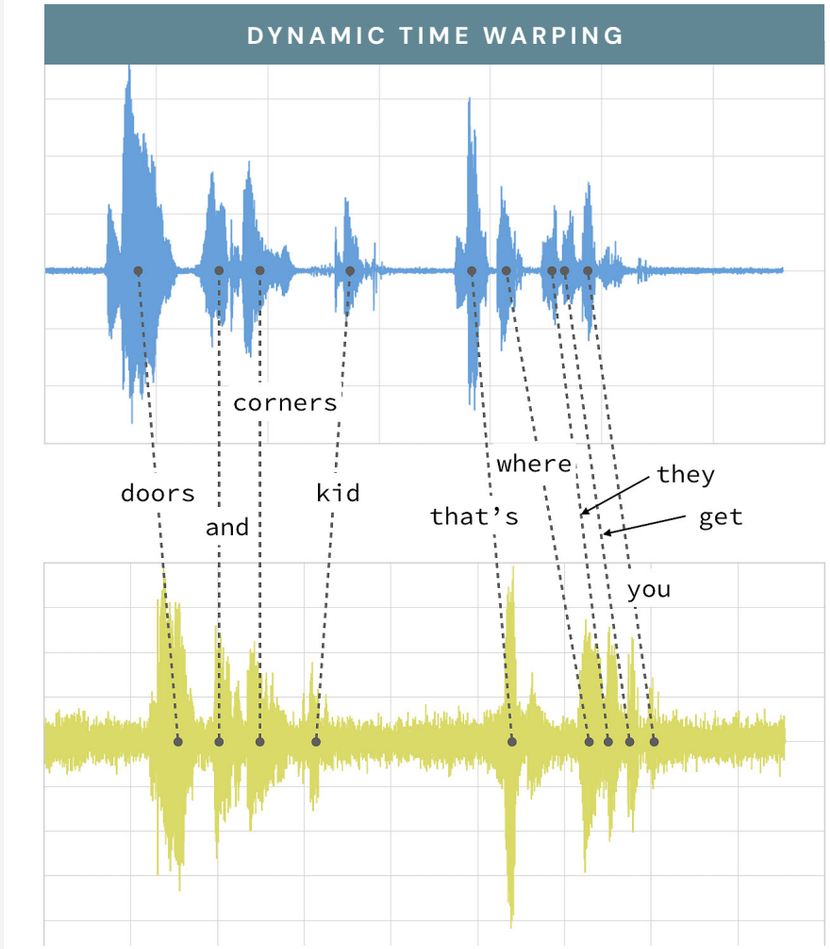
As noted below, the two clips (in this case, clips 1 and 4) have different intonations (amplitude) and latencies for the same quote.



If we were to follow a traditional Euclidean matching (per the following graph), even if we were to discount the amplitudes, the timings between the original clip (blue) and the new clip (yellow) do not match.



With dynamic time warping, we can shift time to allow for a time series comparison between these two clips.

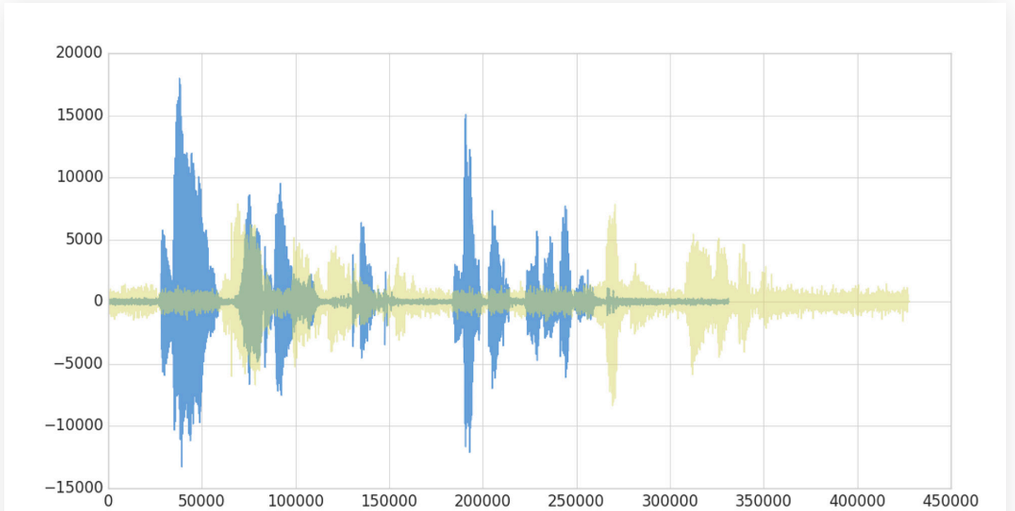


For our time series comparison, we will use the `fastdtw` PyPi library; the instructions to install PyPi libraries within your Databricks workspace can be found here: Azure | AWS. By using fastdtw, we can quickly calculate the distance between the different time series.

```
from fastdtw import fastdtw

# Distance between clip 1 and clip 2
distance = fastdtw(data_clip1, data_clip2)[0]
print("The distance between the two clips is %s" % distance)
```

The full code base can be found in the notebook Dynamic Time Warping Background.

BASE	QUERY	DISTANCE
Clip 1	Clip 2	480148446.0
	Clip 3	310038909.0
	Clip 4	293547478.0



Some quick observations:

- As noted in the preceding graph, clips 1 and 4 have the shortest distance, as the audio clips have the same words and intonations
- The distance between clips 1 and 3 is also quite short (though longer than when compared to clip 4) — even though they have different words, they are using the same intonation and speed
- Clips 1 and 2 have the longest distance due to the extremely exaggerated intonation and speed even though they are using the same quote

As you can see, with dynamic time warping, one can ascertain the similarity of two different time series.

Next

Now that we have discussed dynamic time warping, let's apply this use case to detect sales trends.

CHAPTER 4:

Using Dynamic Time Warping and MLflow to Detect Sales Trends

Part 2 of our Using Dynamic Time Warping and MLflow to Detect Sales Trends series

By **Ricardo Portilla**, **Brenner Heintz** and **Denny Lee**

Try this notebook series (in DBC format) in Databricks →

Background

Imagine that you own a company that creates 3D printed products. Last year, you knew that drone propellers were showing very consistent demand, so you produced and sold those, and the year before you sold phone cases. The new year is arriving very soon, and you're sitting down with your manufacturing team to figure out what your company should produce for next year. Buying the 3D printers for your warehouse put you deep into debt, so you have to make sure that your printers are running at or near 100% capacity at all times in order to make the payments on them.

Since you're a wise CEO, you know that your production capacity over the next year will ebb and flow — there will be some weeks when your production capacity is higher than others. For example, your capacity might be higher during the summer (when you hire seasonal workers), and lower during the third week of every month (because of issues with the 3D printer filament supply chain). Take a look at the chart below to see your company's production capacity estimate:

Your job is to choose a product for which weekly demand meets your production capacity as closely as possible. You're looking over a catalog of products which includes last year's sales numbers for each product, and you think this year's sales will be similar.

If you choose a product with weekly demand that exceeds your production capacity, then you'll have to cancel customer orders, which isn't good for business. On the other hand, if you choose a product without enough weekly demand, you won't be able to keep your printers running at full capacity and may fail to make the debt payments.

Dynamic time warping comes into play here because sometimes supply and demand for the product you choose will be slightly out of sync. There will be some weeks when you simply don't have enough capacity to meet all of your demand, but as long as you're very close and you can make up for it by producing more products in the week or two before or after, your customers won't mind. If we limited ourselves to comparing the sales data with our production capacity using Euclidean matching, we might choose a product that didn't account for this and leave money on the table. Instead, we'll use dynamic time warping to choose the product that's right for your company this year.

Load the product sales data set

We will use the weekly sales transaction data set found in the UCI Data Set Repository to perform our sales-based time series analysis. (Source attribution: James Tan, jamestansc@suss.edu.sg, Singapore University of Social Sciences)

```
import pandas as pd

# Use Pandas to read this data
sales_pdf = pd.read_csv(sales_dbfspath, header='infer')

# Review data
display(spark.createDataFrame(sales_pdf))
```

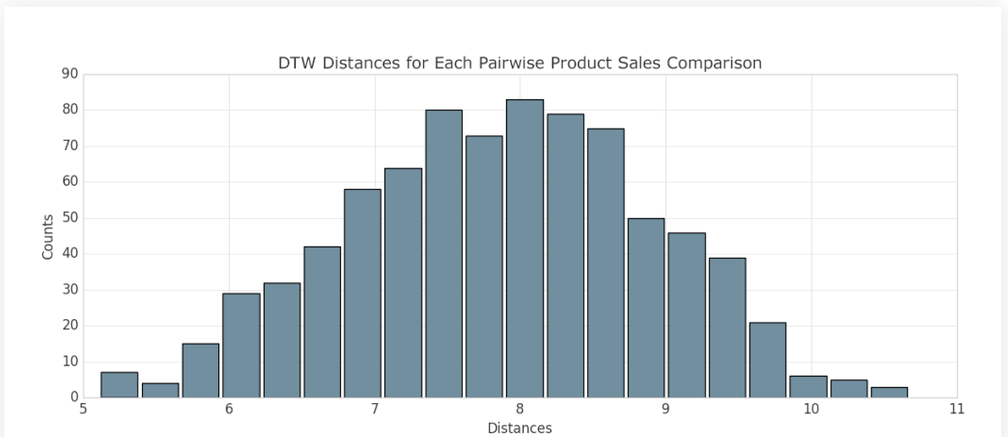
Product_Code	W0	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13
P1	11	12	10	8	13	12	14	21	6	14	11	14	16	9
P2	7	6	3	2	7	1	6	3	3	3	2	2	6	2
P3	7	11	8	9	10	8	7	13	12	6	14	9	4	7
P4	12	8	13	5	9	6	9	13	13	11	8	4	5	4
P5	8	5	13	11	6	7	9	14	9	9	11	18	8	4
P6	3	3	2	7	6	3	8	6	6	3	1	1	5	4
P7	4	8	3	7	8	7	2	3	10	3	5	2	3	4
P8	8	6	10	9	6	8	7	5	10	10	8	8	15	9

Each product is represented by a row, and each week in the year is represented by a column. Values represent the number of units of each product sold per week. There are 811 products in the data set.

Calculate distance to optimal time series by product code

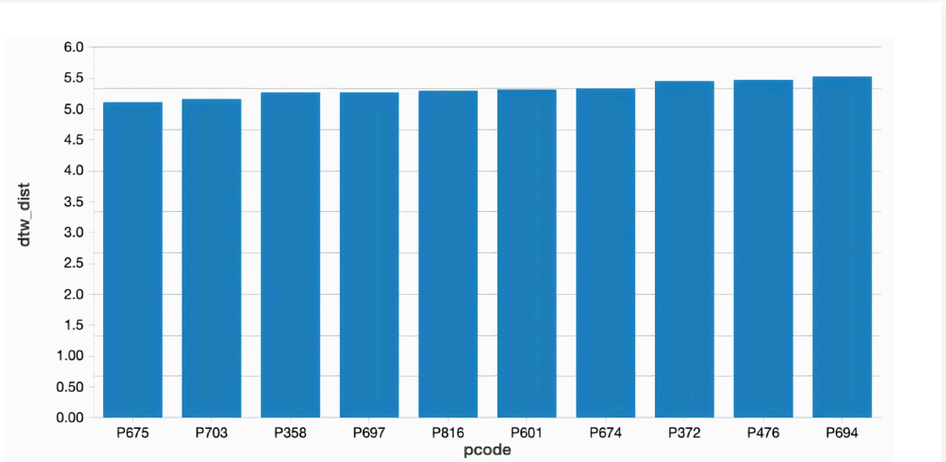
```
# Calculate distance via dynamic time warping between product code and
optimal time series
import numpy as np
import _ucrdtw

def get_keyed_values(s):
    return(s[0], s[1:])

def compute_distance(row):
    return(row[0], _ucrdtw.ucrdtw(list(row[1][0:52]), list(optimal_
pattern), 0.05, True)[1])

ts_values = pd.DataFrame(np.apply_along_axis(get_keyed_values, 1,
sales_pdf.values))
distances = pd.DataFrame(np.apply_along_axis(compute_distance, 1, ts_
values.values))
distances.columns = ['pcode', 'dtw_dist']
```

Using the calculated dynamic time warping "distances" column, we can view the distribution of DTW distances in a histogram.

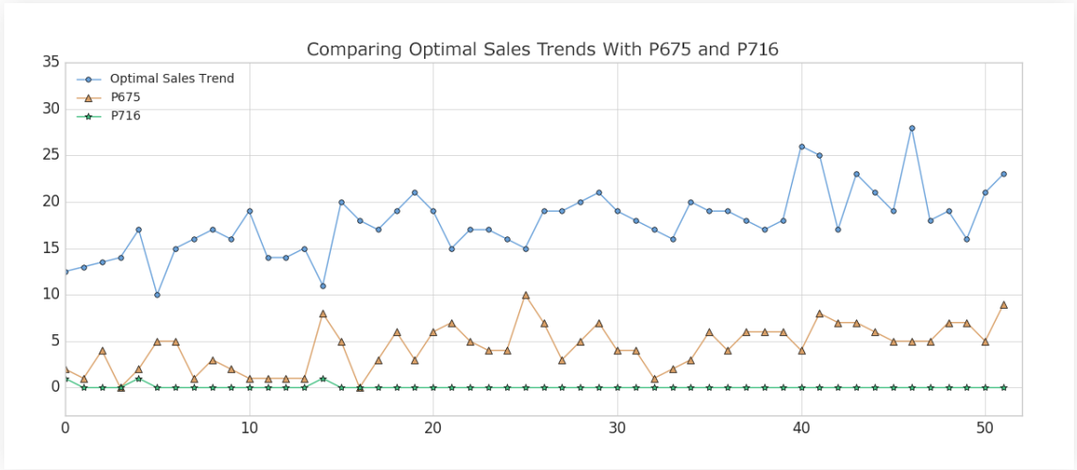


From there, we can identify the product codes closest to the optimal sales trend (i.e., those that have the smallest calculated DTW distance). Since we're using Databricks, we can easily make this selection using a SQL query. Let's display those that are closest.

```
%sql
-- Top 10 product codes closest to the optimal sales trend
select pcode, cast(dtw_dist as float) as dtw_dist from distances order
by cast(dtw_dist as float) limit 10
```



After running this query, along with the corresponding query for the product codes that are *furthest* from the optimal sales trend, we were able to identify the two products that are closest and furthest from the trend. Let's plot both of those products and see how they differ.

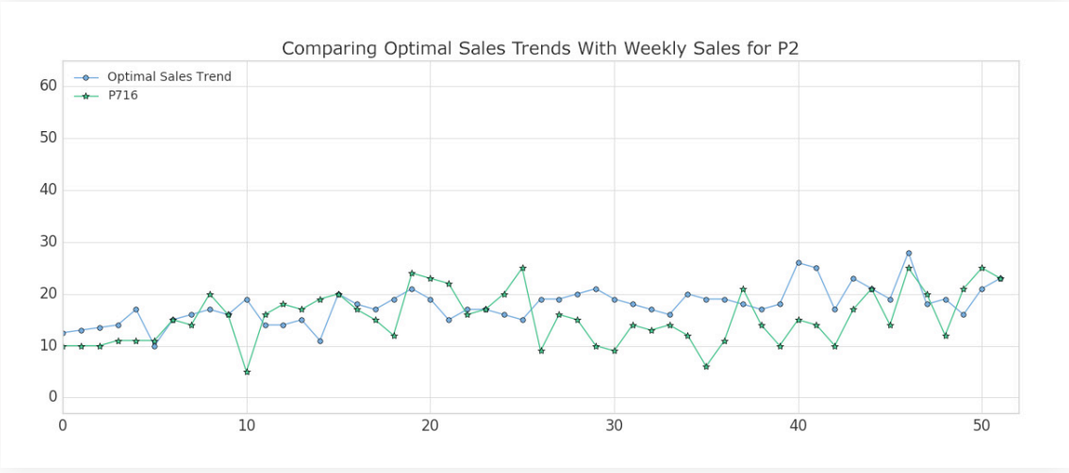


As you can see, Product #675 (shown in the orange triangles) represents the best match to the optimal sales trend, although the absolute weekly sales are lower than we'd like (we'll remedy that later). This result makes sense since we'd expect the product with the closest DTW distance to have peaks and valleys that somewhat mirror the metric we're comparing it to. (Of course, the exact time index for the product would vary on a week-by-week basis due to dynamic time warping.) Conversely, Product #716 (shown in the green stars) is the product with the worst match, showing almost no variability.

Finding the optimal product: Small DTW distance and similar absolute sales numbers

Now that we've developed a list of products that are closest to our factory's projected output (our "optimal sales trend"), we can filter them down to those that have small DTW distances as well as similar absolute sales numbers. One good candidate would be Product #202, which has a DTW distance of 6.86 versus the population median distance of 7.89 and tracks our optimal trend very closely.

```
# Review P202 weekly sales
y_p202 = sales_pdf[sales_pdf['Product_Code'] == 'P202'].values[0][1:53]
```



Using MLflow to track best and worst products, along with artifacts

MLflow is an open source platform for managing the machine learning lifecycle, including experimentation, reproducibility and deployment. **Databricks notebooks offer a fully integrated MLflow environment, allowing you to create experiments, log parameters and metrics, and save results.** For more information about getting started with MLflow, take a look at the excellent documentation.

MLflow's design is centered around the ability to log all of the inputs and outputs of each experiment we do in a systematic, reproducible way. On every pass through the data, known as a "run," we're able to log our experiment's:

- **Parameters:** The inputs to our model
- **Metrics:** The output of our model, or measures of our model's success
- **Artifacts:** Any files created by our model — for example, PNG plots or CSV data output
- **Models:** The model itself, which we can later reload and use to serve predictions

In our case, we can use it to run the dynamic time warping algorithm several times over our data while changing the "stretch factor," the maximum amount of warp that can be applied to our time series data. To initiate an MLflow experiment, and allow for easy logging using `mlflow.log_param()`, `mlflow.log_metric()`, `mlflow.log_artifact()`, and `mlflow.log_model()`, we wrap our main function using:

```
iwith mlflow.start_run() as run:
    ...
```

as shown in the abbreviated code at right.

```
import mlflow

def run_DTW(ts_stretch_factor):
    # calculate DTW distance and Z-score for each product
    <strong>with mlflow.start_run() as run:</strong>

        # Log Model using Custom Flavor
        dtw_model = {'stretch_factor' : float(ts_stretch_factor),
'pattern' : optimal_pattern}
        <strong>mlflow_custom_flavor.log_model(dtw_model, artifact_
path="model")</strong>

        # Log our stretch factor parameter to MLflow
        <strong>mlflow.log_param("stretch_factor", ts_stretch_factor)</
strong>

        # Log the median DTW distance for this run
        <strong>mlflow.log_metric("Median Distance", distance_median)</
strong>

        # Log artifacts - CSV file and PNG plot - to MLflow
        <strong>mlflow.log_artifact('zscore_outliers_' + str(ts_stretch_
factor) + '.csv')
        mlflow.log_artifact('DTW_dist_histogram.png')

    return run.info</strong>

stretch_factors_to_test = [0.0, 0.01, 0.025, 0.05, 0.1, 0.25, 0.5]
for n in stretch_factors_to_test:
    run_DTW(n)
```

With each run through the data, we've created a log of the "stretch factor" parameter being used, and a log of products we classified as being outliers based upon the Z-score of the DTW distance metric. We were even able to save an artifact (file) of a histogram of the DTW distances. These experimental runs are saved locally on Databricks and remain accessible in the future if you decide to view the results of your experiment at a later date.

Now that MLflow has saved the logs of each experiment, we can go back through and examine the results. From your Databricks notebook, select the "Runs" icon in the upper right-hand corner to view and compare the results of each of our runs.

www.youtube.com/watch?v=62PAPZo-2ZU

Not surprisingly, as we increase our "stretch factor," our distance metric decreases. Intuitively, this makes sense: as we give the algorithm more flexibility to warp the time indices forward or backward, it will find a closer fit for the data. In essence, we've traded some bias for variance.

Logging models in MLflow

MLflow has the ability to not only log experiment parameters, metrics and artifacts (like plots or CSV files), but also to log machine learning models. An MLflow model is simply a folder that is structured to conform to a consistent API, ensuring compatibility with other MLflow tools and features. This interoperability is very powerful, allowing any Python model to be rapidly deployed to many different types of production environments.

MLflow comes pre-loaded with a number of common model "flavors" for many of the most popular machine learning libraries, including scikit-learn, Spark MLlib, PyTorch, TensorFlow, and others. These model flavors make it trivial to log and reload models after they are initially constructed, as demonstrated in this blog post. For example, when using MLflow with scikit-learn, logging a model is as easy as running the following code from within an experiment:

```
mlflow.sklearn.log_model(model=sk_model, artifact_path="sk_model_path")
```

MLflow also offers a "Python function" flavor, which allows you to save any model from a third-party library (such as XGBoost or spaCy), or even a simple Python function itself, as an MLflow model. Models created using the Python function flavor live within the same ecosystem and are able to interact with other MLflow tools through the Inference API. Although it's impossible to plan for every use case, the Python function model flavor was designed to be as universal and flexible as possible. It allows for custom processing and logic evaluation, which can come in handy for ETL applications. Even as more "official" model flavors come online, the generic Python function flavor will still serve as an important "catchall," providing a bridge between Python code of any kind and MLflow's robust tracking toolkit.

Logging a model using the Python function flavor is a straightforward process. **Any model or function can be saved as a model, with one requirement: It must take in a pandas DataFrame as input, and return a DataFrame or NumPy array.** Once that requirement is met, saving your function as an MLflow model involves defining a Python class that inherits from PythonModel, and overriding the `.predict() method` with your custom function, as described here**.**

Loading a logged model from one of our runs

Now that we've run through our data with several different stretch factors, the natural next step is to examine our results and look for a model that did particularly well according to the metrics that we've logged. MLflow makes it easy to then reload a logged model, and use it to make predictions on new data, using the following instructions:

1. Click on the link for the run you'd like to load our model from
2. Copy the "Run ID"
3. Make note of the name of the folder the model is stored in. In our case, it's simply named "model"
4. Enter the model folder name and Run ID as shown below:

```
import custom_flavor as mlflow_custom_flavor

loaded_model = mlflow_custom_flavor.load_model(artifact_path='model',
run_id='e26961b25c4d4402a9a5a7a679fc8052')
```

To show that our model is working as intended, we can now load the model and use it to measure DTW distances on two new products that we've created within the variable `new_sales_units` :

```
# use the model to evaluate new products found in 'new_sales_units'
output = loaded_model.predict(new_sales_units)
print(output)
```

Next steps

As you can see, our MLflow model is predicting new and unseen values with ease. And since it conforms to the Inference API, we can deploy our model on any serving platform (such as Microsoft Azure ML or Amazon SageMaker), deploy it as a local REST API end point, or create a user-defined function (UDF) that can easily be used with Spark SQL. In closing, we demonstrated how we can use dynamic time warping to predict sales trends using the Databricks Unified Data Analytics Platform. Try out the Using Dynamic Time Warping and MLflow to Predict Sales Trends notebook with Databricks Runtime for Machine Learning today.

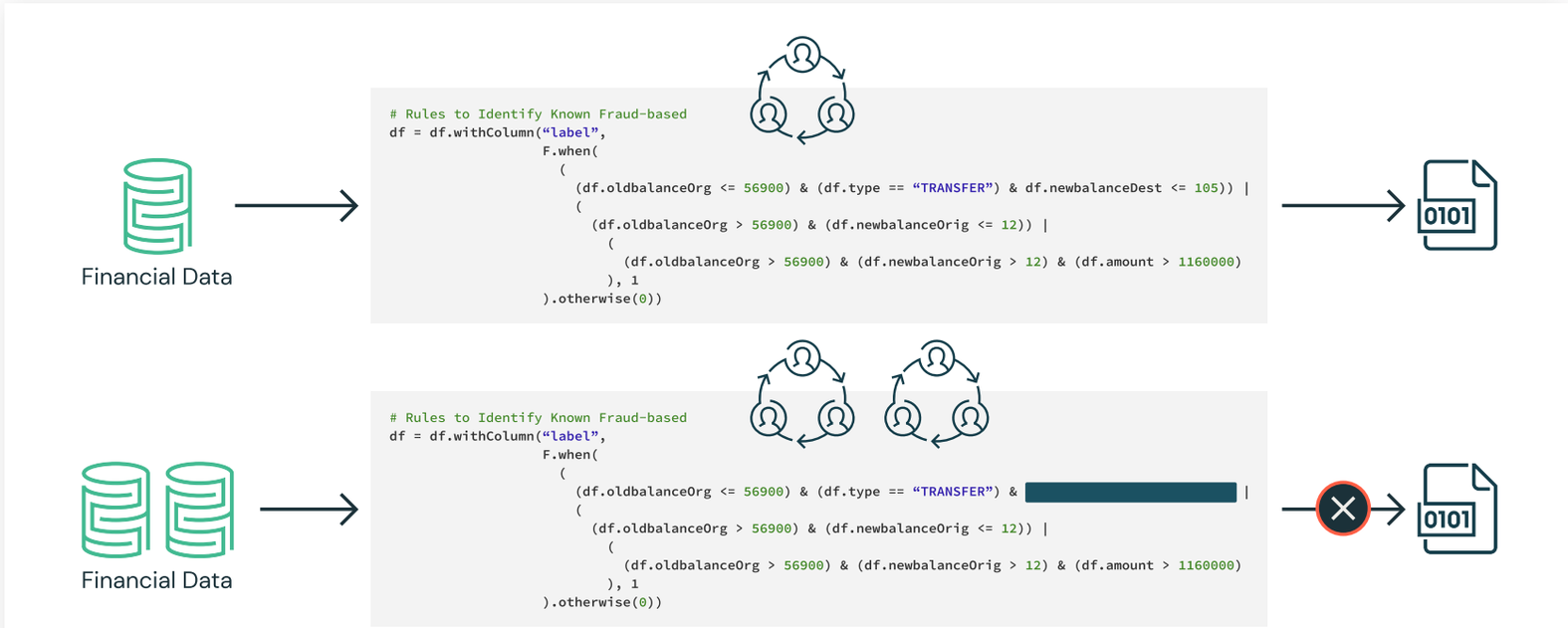
CHAPTER 5:

Detecting Financial Fraud at Scale With Decision Trees and MLflow on Databricks

By **Elena Boiarskaia**, **Navin Albert** and **Denny Lee**

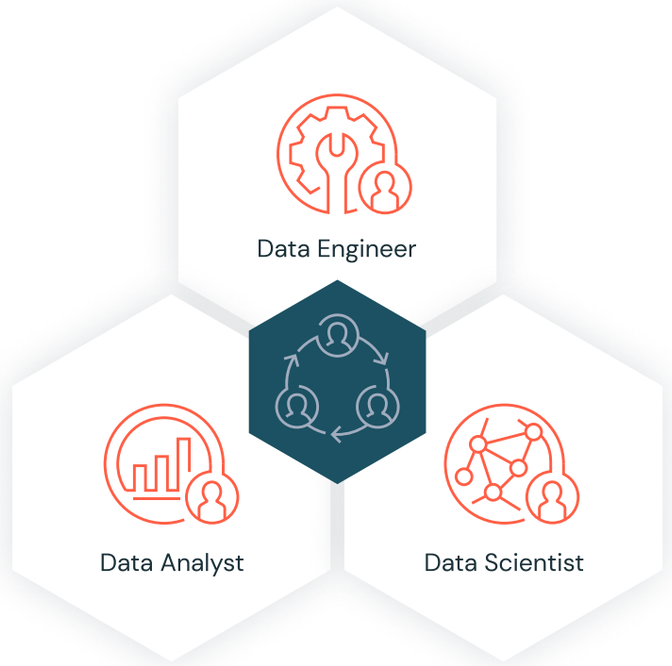
Try this notebook in Databricks →

Detecting fraudulent patterns at scale using artificial intelligence is a challenge, no matter the use case. The massive amounts of historical data to sift through, the complexity of the constantly evolving machine learning and deep learning techniques, and the very small number of actual examples of fraudulent behavior are comparable to finding a needle in a haystack while not knowing what the needle looks like. In the financial services industry, the added concerns with security and the importance of explaining how fraudulent behavior was identified further increase the complexity of the task.



To build these detection patterns, a team of domain experts comes up with a set of rules based on how fraudsters typically behave. A workflow may include a subject matter expert in the financial fraud detection space putting together a set of requirements for a particular behavior. A data scientist may then take a subsample of the available data and select a set of deep learning or machine learning algorithms using these requirements and possibly some known fraud cases. To put the pattern in production, a data engineer may convert the resulting model to a set of rules with thresholds, often implemented using SQL.

This approach allows the financial institution to present a clear set of characteristics that lead to the identification of a fraudulent transaction that is compliant with the General Data Protection Regulation (GDPR). However, this approach also poses numerous difficulties. The implementation of a fraud detection system using a hardcoded set of rules is very brittle. Any changes to the fraud patterns would take a very long time to update. This, in turn, makes it difficult to keep up with and adapt to the shift in fraudulent activities that are happening in the current marketplace.

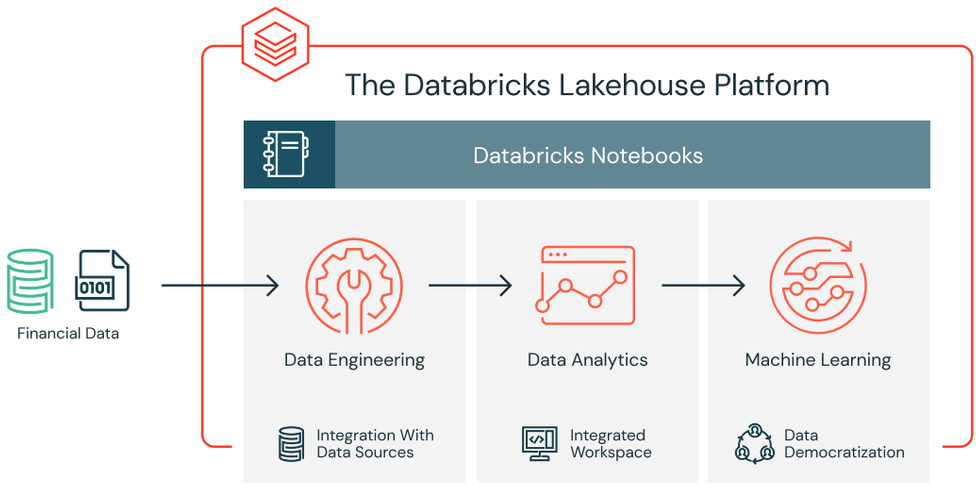


Additionally, the systems in the workflow described above are often siloed, with the domain experts, data scientists and data engineers all compartmentalized. The data engineer is responsible for maintaining massive amounts of data and translating the work of the domain experts and data scientists into production level code. Due to a lack of a common platform, the domain experts and data scientists have to rely on sampled down data that fits on a single machine for analysis. This leads to difficulty in communication and ultimately a lack of collaboration.

In this blog, we will showcase how to convert several such rule-based detection use cases to machine learning use cases on the Databricks platform, unifying the key players in fraud detection: domain experts, data scientists and data engineers. We will learn how to create a machine learning fraud detection data pipeline and visualize the data in real time, leveraging a framework for building modular features from large data sets. We will also learn how to detect fraud using decision trees and Apache Spark™ MLlib. We will then use MLflow to iterate and refine the model to improve its accuracy.

Solving with machine learning

There is a certain degree of reluctance with regard to machine learning models in the financial world, as they are believed to offer a "black box" solution with no way of justifying the identified fraudulent cases. GDPR requirements, as well as financial regulations, make it seemingly impossible to leverage the power of data science. However, several successful use cases have shown that applying machine learning to detect fraud at scale can solve a host of the issues mentioned above.



Training a supervised machine learning model to detect financial fraud is very difficult due to the low number of actual confirmed examples of fraudulent behavior. However, the presence of a known set of rules that identify a particular type of fraud can help create a set of synthetic labels and an initial set of features. The output of the detection pattern that has been developed by the domain experts in the field has likely gone through the appropriate approval process to be put in production. It produces the expected fraudulent behavior flags and may, therefore, be used as a starting point to train a machine learning model.

This simultaneously mitigates three concerns:

1. The lack of training labels
2. The decision of what features to use
3. Having an appropriate benchmark for the model

Training a machine learning model to recognize the rule-based fraudulent behavior flags offers a direct comparison with the expected output via a confusion matrix. Provided that the results closely match the rule-based detection pattern, this approach helps gain confidence in machine learning–based fraud prevention with the skeptics. The output of this model is very easy to interpret and may serve as a baseline discussion of the expected false negatives and false positives when compared to the original detection pattern.

Furthermore, the concern with machine learning models being difficult to interpret may be further assuaged if a decision tree model is used as the initial machine learning model. Because the model is being trained to a set of rules, the decision tree is likely to outperform any other machine learning model. The additional benefit is, of course, the utmost transparency of the model, which will essentially show the decision-making process for fraud, but without human intervention and the need to hard code any rules or thresholds. Of course, it must be understood that the future iterations of the model may utilize a different algorithm altogether to achieve maximum accuracy. The transparency of the model is ultimately achieved by understanding the features that went into the algorithm. Having interpretable features will yield interpretable and defensible model results.

The biggest benefit of the machine learning approach is that after the initial modeling effort, future iterations are modular, and updating the set of labels, features or model type is very easy and seamless, reducing the time to production. This is further facilitated on the Databricks Collaborative Notebooks where the domain experts, data scientists and data engineers may work off the same data set at scale and collaborate directly in the notebook environment. So let's get started!

Ingesting and exploring the data

We will use a synthetic data set for this example. To load the data set yourself, please download it to your local machine from Kaggle and then import the data via Import Data — Azure and AWS.

The PaySim data simulates mobile money transactions based on a sample of real transactions extracted from one month of financial logs from a mobile money service implemented in an African country. The below table shows the information that the data set provides:

Column Name	Description
step	maps a unit of time in the real world. In this case 1 step is 1 hour of time. Total steps 744 (30 days simulation).
type	CASH-IN, CASH-OUT, DEBIT, PAYMENT and TRANSFER.
amount	amount of the transaction in local currency.
nameOrig	customer who started the transaction
oldbalanceOrg	initial balance before the transaction
newbalanceOrig	new balance after the transaction
nameDest	customer who is the recipient of the transaction
oldbalanceDest	initial balance recipient before the transaction. Note that there is not information for customers that start with M (Merchants).
newbalanceDest	new balance recipient after the transaction. Note that there is not information for customers that start with M (Merchants).

Exploring the data

Creating the DataFrames: Now that we have uploaded the data to Databricks File System (DBFS), we can quickly and easily create DataFrames using Spark SQL.

```
# Create df DataFrame which contains our simulated financial fraud detection dataset
df = spark.sql("select step, type, amount, nameOrig, oldbalanceOrg, newbalanceOrig, nameDest, oldbalanceDest, newbalanceDest from sim_fin_fraud_detection")
```

Now that we have created the DataFrame, let's take a look at the schema and the first thousand rows to review the data.

```
# Review the schema of your data
df.printSchema()
root
|-- step: integer (nullable = true)
|-- type: string (nullable = true)
|-- amount: double (nullable = true)
|-- nameOrig: string (nullable = true)
|-- oldbalanceOrg: double (nullable = true)
|-- newbalanceOrig: double (nullable = true)
|-- nameDest: string (nullable = true)
|-- oldbalanceDest: double (nullable = true)
|-- newbalanceDest: double (nullable = true)
```

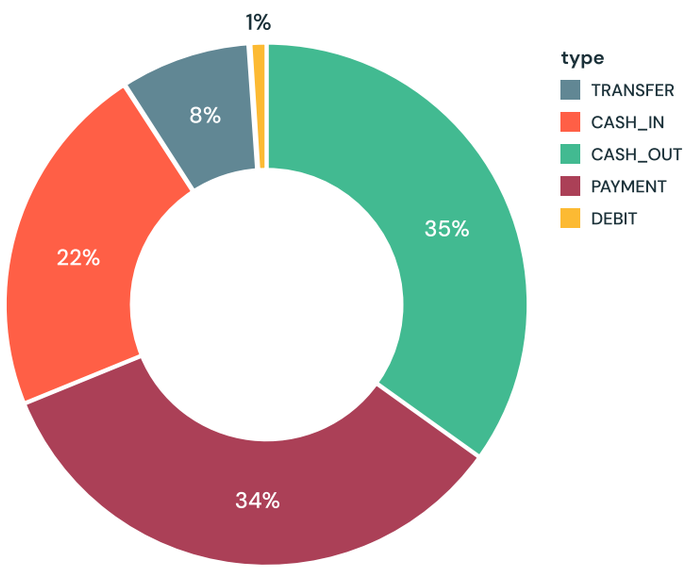
1	PAYMENT	7107.77	C154988899	183195	176087.23	M408069119	0
1	PAYMENT	7861.64	C1912850431	176087.23	168225.59	M633326333	0
1	PAYMENT	4024.36	C1265012928	2671	0	M1176932104	0

Showing the first 1000 rows.

Types of transactions

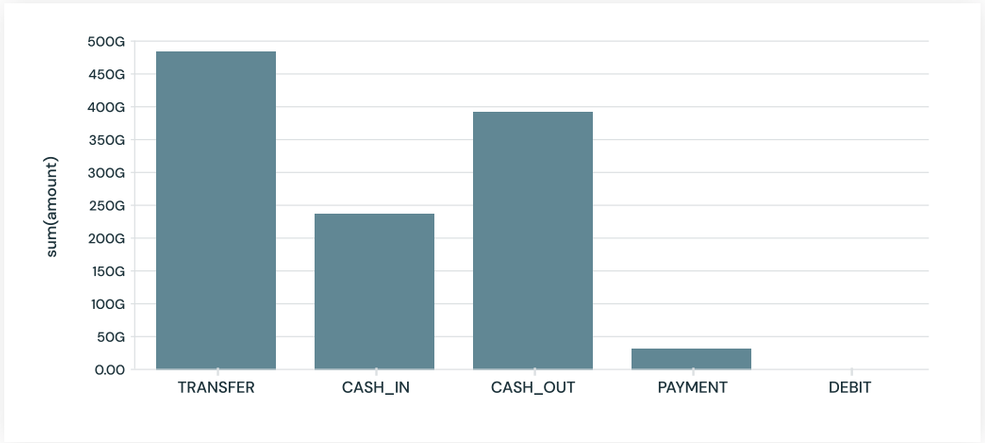
Let's visualize the data to understand the types of transactions the data captures and their contribution to the overall transaction volume.

```
%sql
-- Organize by Type
select type, count(1) from financials group by type
```



To get an idea of how much money we are talking about, let's also visualize the data based on the types of transactions and on their contribution to the amount of cash transferred (i.e., sum(amount)).

```
%sql
select type, sum(amount) from financials group by type
```



Rule-based model

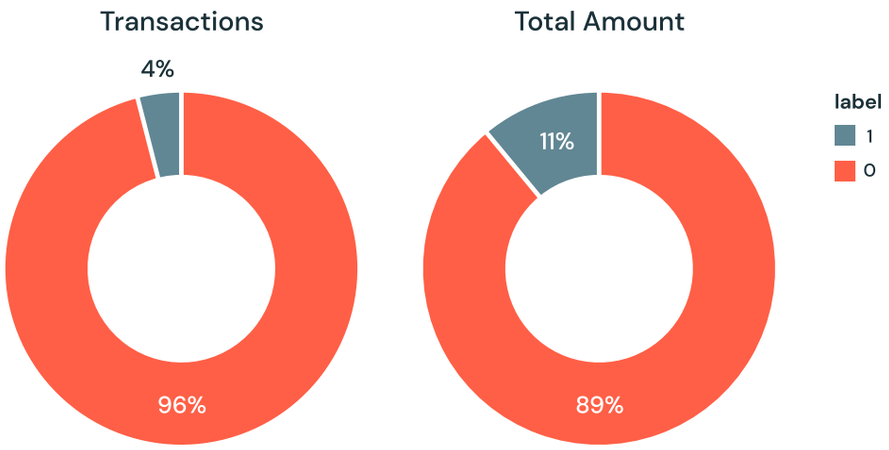
We are not likely to start with a large data set of known fraud cases to train our model. In most practical applications, fraudulent detection patterns are identified by a set of rules established by the domain experts. Here, we create a column called `label` based on these rules.

```
# Rules to Identify Known Fraud-based
df = df.withColumn("label",
                   F.when(
                     (
                       (df.oldbalanceOrg  56900) & (df.newbalanceOrig
56900) & (df.newbalanceOrig > 12) & (df.amount > 1160000)
                                ), 1
                   ).otherwise(0))
```

Visualizing data flagged by rules

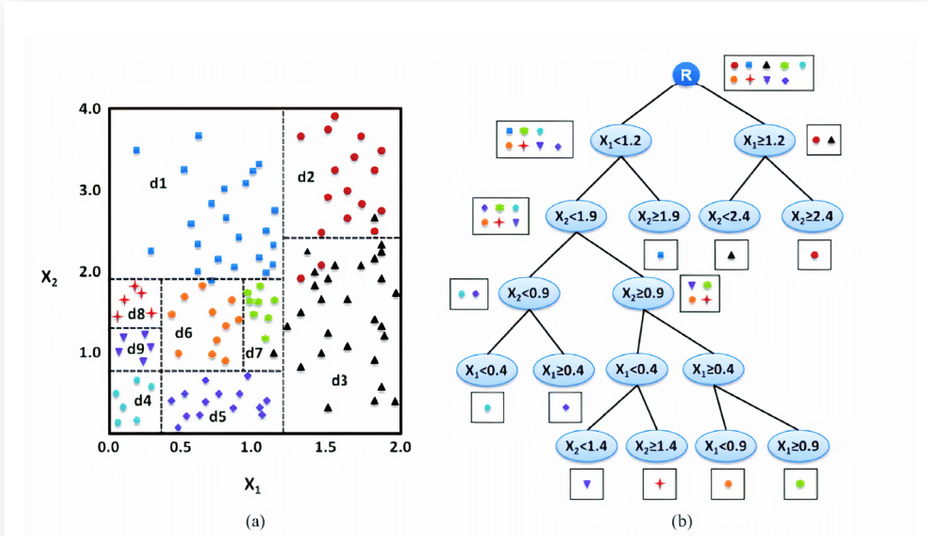
These rules often flag quite a large number of fraudulent cases. Let's visualize the number of flagged transactions. We can see that the rules flag about 4% of the cases and 11% of the total dollar amount as fraudulent.

```
%sql
select label, count(1) as 'Transactions', sun(amount) as 'Total Amount'
from financials_labeled group by label
```



Selecting the appropriate machine learning models

In many cases, a black box approach to fraud detection cannot be used. First, the domain experts need to be able to understand why a transaction was identified as fraudulent. Then, if action is to be taken, the evidence has to be presented in court. The decision tree is an easily interpretable model and is a great starting point for this use case.



Creating the training set

To build and validate our ML model, we will do an 80/20 split using `.randomSplit.` This will set aside a randomly chosen 80% of the data for training and the remaining 20% to validate the results.

```
# Split our dataset between training and test datasets
(train, test) = df.randomSplit([0.8, 0.2], seed=12345)
```

Creating the ML model pipeline

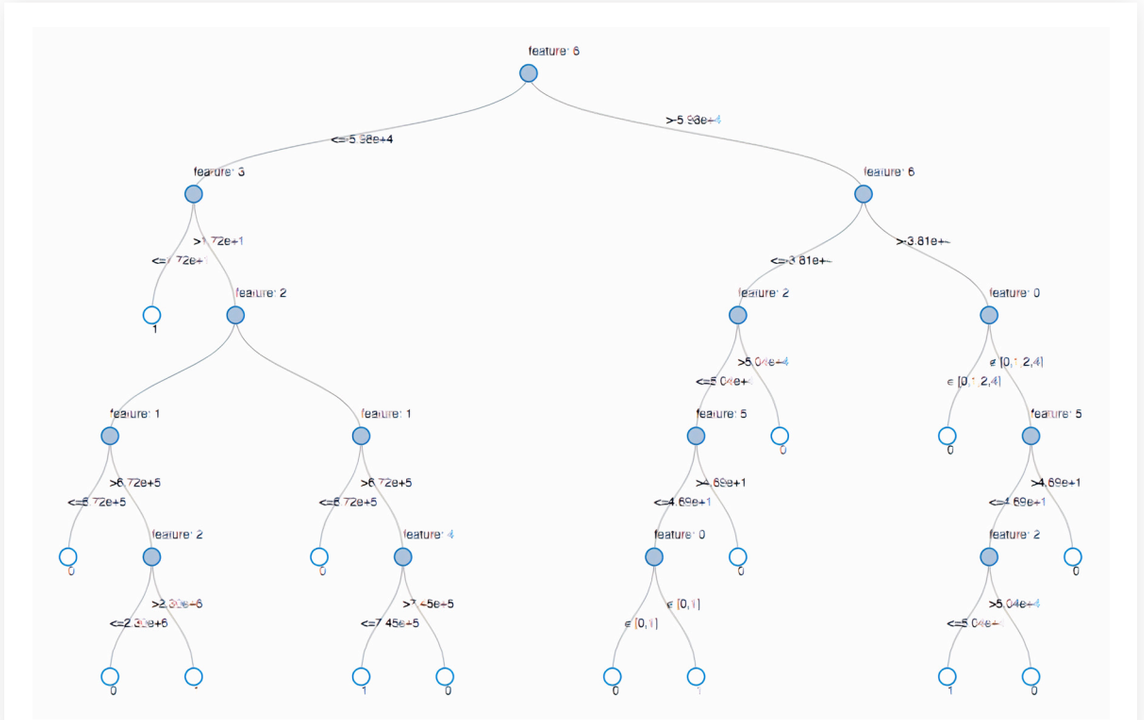
To prepare the data for the model, we must first convert categorical variables to numeric using `.StringIndexer.` We then must assemble all of the features we would like for the model to use. We create a pipeline to contain these feature preparation steps in addition to the decision tree model so that we may repeat these steps on different data sets. Note that we fit the pipeline to our training data first and will then use it to transform our test data in a later step.

```
from pyspark.ml import Pipeline
from pyspark.ml.feature import StringIndexer
from pyspark.ml.feature import VectorAssembler
from pyspark.ml.classification import DecisionTreeClassifier

# Encodes a string column of labels to a column of label indices
indexer = StringIndexer(inputCol = "type", outputCol = "typeIndexed")

# VectorAssembler is a transformer that combines a given list of
columns into a single vector column
va = VectorAssembler(inputCols = ["typeIndexed", "amount",
"oldbalanceOrg", "newbalanceOrig", "oldbalanceDest", "newbalanceDest",
"orgDiff", "destDiff"], outputCol = "features")

# Using the DecisionTree classifier model
dt = DecisionTreeClassifier(labelCol = "label", featuresCol =
"features", seed = 54321, maxDepth = 5)

# Create our pipeline stages
pipeline = Pipeline(stages=[indexer, va, dt])

# View the Decision Tree model (prior to CrossValidator)
dt_model = pipeline.fit(train)
```

Visualizing the model

Calling `display()` on the last stage of the pipeline, which is the decision tree model, allows us to view the initial fitted model with the chosen decisions at each node. This helps us to understand how the algorithm arrived at the resulting predictions.

```
display(dt_model.stages[-1])
```



Visual representation of the decision tree model

Model tuning

To ensure we have the best-fitting tree model, we will cross-validate the model with several parameter variations. Given that our data consists of 96% negative and 4% positive cases, we will use the Precision-Recall (PR) evaluation metric to account for the unbalanced distribution.

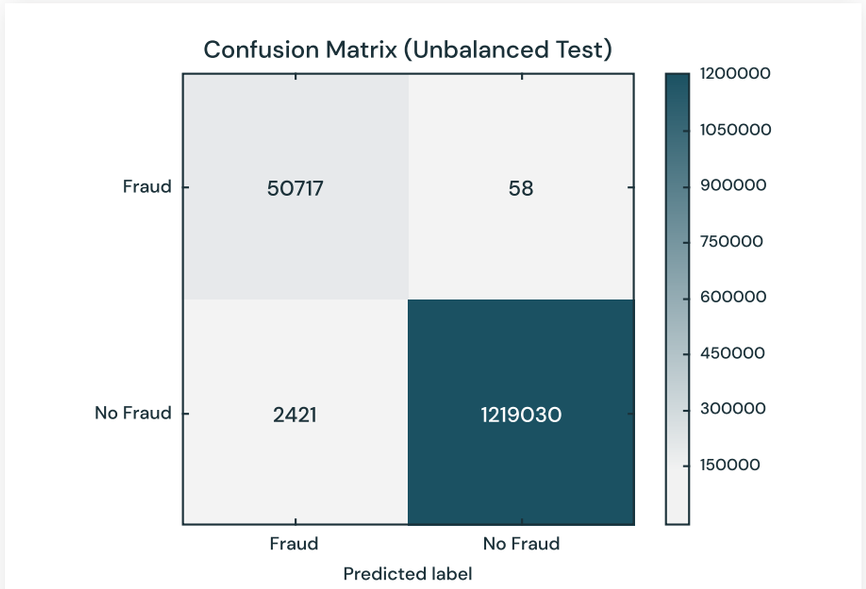
```
<b>from</b> pyspark.ml.tuning <b>import</b> CrossValidator,
ParamGridBuilder

# Build the grid of different parameters
paramGrid = ParamGridBuilder() \
.addGrid(dt.maxDepth, [5, 10, 15]) \
.addGrid(dt.maxBins, [10, 20, 30]) \
.build()

# Build out the cross validation
crossval = CrossValidator(estimator = dt,
                          estimatorParamMaps = paramGrid,
                          evaluator = evaluatorPR,
                          numFolds = 3)
# Build the CV pipeline
pipelineCV = Pipeline(stages=[indexer, va, crossval])

# Train the model using the pipeline, parameter grid, and preceding
BinaryClassificationEvaluator
cvModel_u = pipelineCV.fit(train)
```

Model performance

We evaluate the model by comparing the Precision-Recall (PR) and area under the ROC curve (AUC) metrics for the training and test sets. Both PR and AUC appear to be very high.

```
# Build the best model (training and test datasets)
train_pred = cvModel_u.transform(train)
test_pred = cvModel_u.transform(test)

# Evaluate the model on training datasets
pr_train = evaluatorPR.evaluate(train_pred)
auc_train = evaluatorAUC.evaluate(train_pred)

# Evaluate the model on test datasets
pr_test = evaluatorPR.evaluate(test_pred)
auc_test = evaluatorAUC.evaluate(test_pred)

# Print out the PR and AUC values
print("PR train:", pr_train)
print("AUC train:", auc_train)
print("PR test:", pr_test)
print("AUC test:", auc_test)

---
# Output:
# PR train: 0.9537894984523128
# AUC train: 0.998647996459481
# PR test: 0.9539170535377599
# AUC test: 0.9984378183482442
```

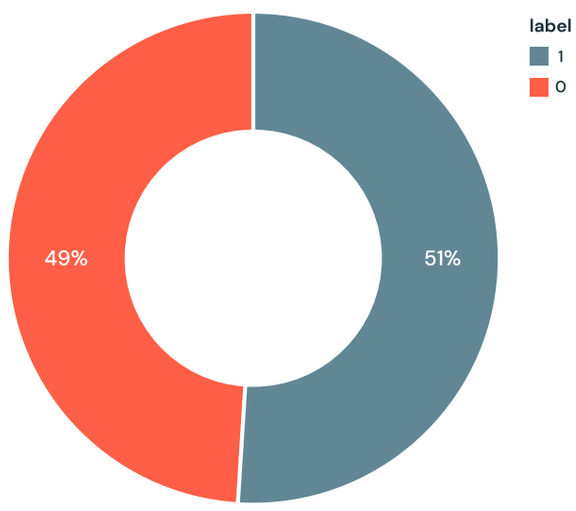
To see how the model misclassified the results, let's use Matplotlib and pandas to visualize our confusion matrix.



Balancing the classes

We see that the model is identifying 2,421 more cases than the original rules identified. This is not as alarming, as detecting more potential fraudulent cases could be a good thing. However, there are 58 cases that were not detected by the algorithm but were originally identified. We are going to attempt to improve our prediction further by balancing our classes using undersampling. That is, we will keep all the fraud cases and then downsample the non-fraud cases to match that number to get a balanced data set. When we visualize our new data set, we see that the yes and no cases are 50/50.

```
# Reset the DataFrames for no fraud (`dfn`) and fraud (`dfy`)
dfn = train.filter(train.label == 0)
dfy = train.filter(train.label == 1)

# Calculate summary metrics
N = train.count()
y = dfy.count()
p = y/N

# Create a more balanced training dataset
train_b = dfn.sample(<b>False</b>, p, seed = 92285).union(dfy)

# Print out metrics
print("Total count: %s, Fraud cases count: %s, Proportion of fraud
cases: %s" % (N, y, p))
print("Balanced training dataset count: %s" % train_b.count())

---
# Output:
# Total count: 5090394, Fraud cases count: 204865, Proportion of fraud
cases: 0.040245411258932016
# Balanced training dataset count: 401898
---

# Display our more balanced training dataset
display(train_b.groupBy("label").count())
```



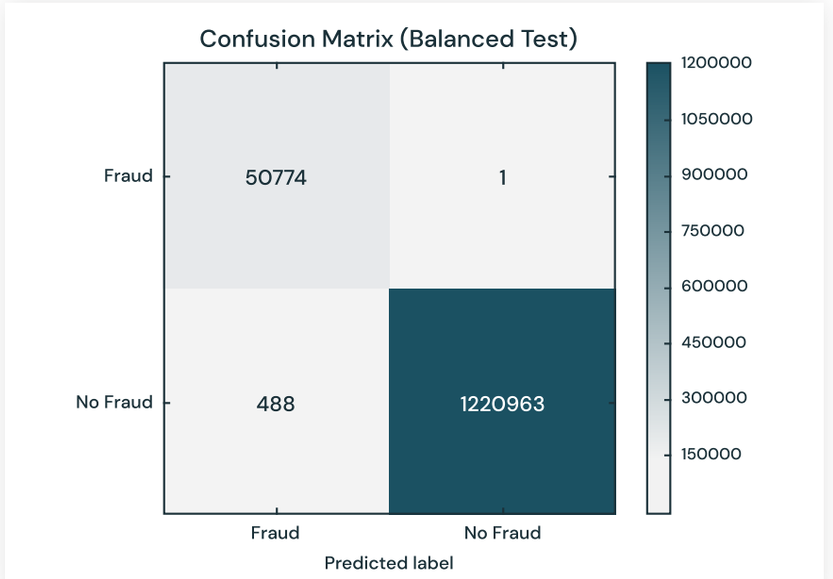
Updating the pipeline

Now let's update the ML pipeline and create a new cross validator. Because we are using ML pipelines, we only need to update it with the new data set and we can quickly repeat the same pipeline steps.

```
# Re-run the same ML pipeline (including parameters grid)
crossval_b = CrossValidator(estimator = dt,
estimatorParamMaps = paramGrid,
evaluator = evaluatorAUC,
numFolds = 3)
pipelineCV_b = Pipeline(stages=[indexer, va, crossval_b])

# Train the model using the pipeline, parameter grid, and
BinaryClassificationEvaluator using the `train_b` dataset
cvModel_b = pipelineCV_b.fit(train_b)

# Build the best model (balanced training and full test datasets)
train_pred_b = cvModel_b.transform(train_b)
test_pred_b = cvModel_b.transform(test)

# Evaluate the model on the balanced training datasets
pr_train_b = evaluatorPR.evaluate(train_pred_b)
auc_train_b = evaluatorAUC.evaluate(train_pred_b)

# Evaluate the model on full test datasets
pr_test_b = evaluatorPR.evaluate(test_pred_b)
auc_test_b = evaluatorAUC.evaluate(test_pred_b)

# Print out the PR and AUC values
print("PR train:", pr_train_b)
print("AUC train:", auc_train_b)
print("PR test:", pr_test_b)
print("AUC test:", auc_test_b)

---
# Output:
# PR train: 0.999629161563572
# AUC train: 0.9998071389056655
# PR test: 0.9904709171789063
# AUC test: 0.9997903902204509
```

Review the results

Now let's look at the results of our new confusion matrix. The model misidentified only one fraudulent case. Balancing the classes seems to have improved the model.



Model feedback and using MLflow

Once a model is chosen for production, we want to continuously collect feedback to ensure that the model is still identifying the behavior of interest. Since we are starting with a rule-based label, we want to supply future models with verified true labels based on human feedback. This stage is crucial for maintaining confidence and trust in the machine learning process. Since analysts are not able to review every single case, we want to ensure we are presenting them with carefully chosen cases to validate the model output. For example, predictions, where the model has low certainty, are good candidates for analysts to review. The addition of this type of feedback will ensure the models will continue to improve and evolve with the changing landscape.

MLflow helps us throughout this cycle as we train different model versions. We can keep track of our experiments, comparing the results of different model configurations and parameters. For example here, we can compare the PR and AUC of the models trained on balanced and unbalanced data sets using the MLflow UI. Data scientists can use MLflow to keep track of the various model metrics and any additional visualizations and artifacts to help make the decision of which model should be deployed in production. The data engineers will then be able to easily retrieve the chosen model along with the library versions used for training as a .jar file to be deployed on new data in production. Thus, the collaboration between the domain experts who review the model results, the data scientists who update the models, and the data engineers who deploy the models in production will be strengthened throughout this iterative process.

> www.youtube.com/watch?v=x_4S9r-Kks8
>
> www.youtube.com/watch?v=BVISypymHzw

Conclusion

We have reviewed an example of how to use a rule-based fraud detection label and convert it to a machine learning model using Databricks with MLflow. This approach allows us to build a scalable, modular solution that will help us keep up with ever-changing fraudulent behavior patterns. Building a machine learning model to identify fraud allows us to create a feedback loop that helps the model to evolve and identify new potential fraudulent patterns. We have seen how a decision tree model, in particular, is a great starting point to introduce machine learning to a fraud detection program due to its interpretability and excellent accuracy.

A major benefit of using the Databricks platform for this effort is that it allows for data scientists, engineers and business users to seamlessly work together throughout the process. Preparing the data, building models, sharing the results and putting the models into production can now happen on the same platform, allowing for unprecedented collaboration. This approach builds trust across the previously siloed teams, leading to an effective and dynamic fraud detection program.

Try this notebook by signing up for a free trial in just a few minutes and get started creating your own models.

CHAPTER 6:

AI Drug Discovery Made Easy: Your Guide to Chemprop on Databricks

Did you know that AI was successfully used to discover a novel antibiotic, halicin, in 2020? This was noteworthy because halicin was structurally unique, highly differentiated from conventional antibiotics like penicillins, and unlocked a new direction in countering growing antibiotic resistance (Stokes et al., 2020).

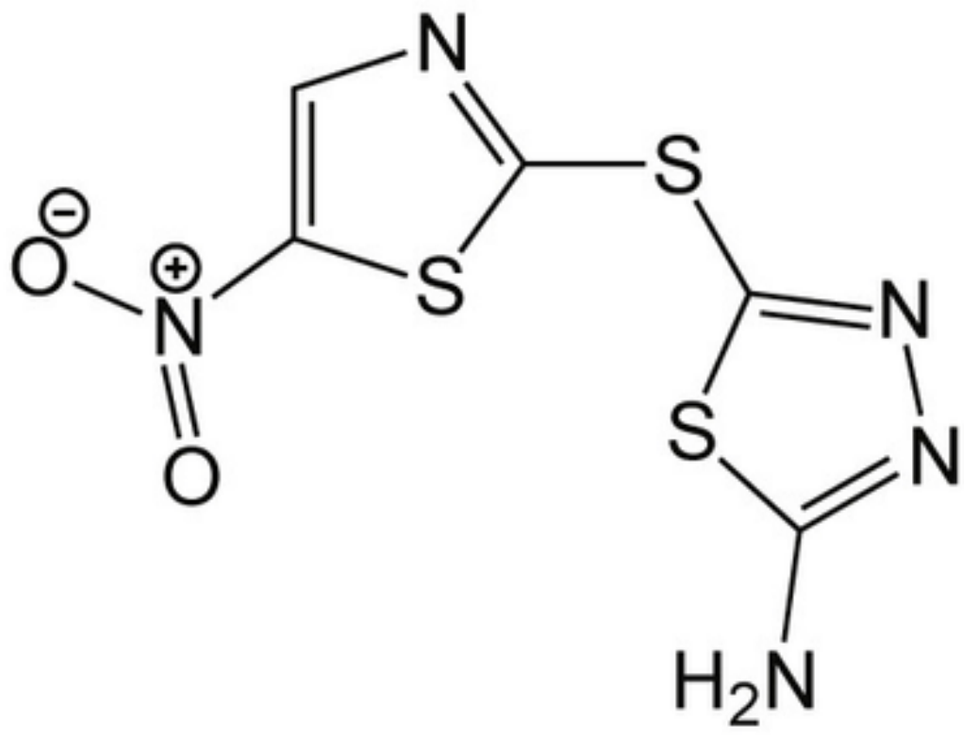


Fig 1. Halicin, a structurally unique and novel antibiotic, discovered using Chemprop

Halicin was discovered using Chemprop (git repo). You can do the same to discover a new drug or a new disease indication for an existing drug (aka drug repurposing) using Chemprop and other open source AI tools on Databricks. This blog shows how highly specialized libraries like Chemprop can be easily integrated into Databricks for drug discovery.

Why do AI drug design on Databricks?

Databricks facilitates production-grade research by providing a unified platform for data processing, model training and deployment.

Its Unity Catalog, which manages data and model assets, promotes discovery and collaboration, making it easy to search and reuse large and complex datasets and models.

MLflow, while open source, is a first-class citizen on Databricks, allowing both no-code and SDK options for experiment tracking, model registration, serving and monitoring. MLflow simplifies MLOps so research scientists can focus on developing models and results interpretation.

Why use Chemprop?

Chemprop is a suite of AI tools based on a directed message-passing neural network (MPNN), which treats molecules as graphs (atoms as nodes and bonds as edges). The model applies a series of message-passing steps where it aggregates information from neighboring atoms and bonds to build an understanding of local chemistry. This learned fingerprint representation is fed into a feed-forward neural network (FFN) that outputs a molecular property such as toxicity, or in halicin's case, the ability to inhibit bacterial growth.

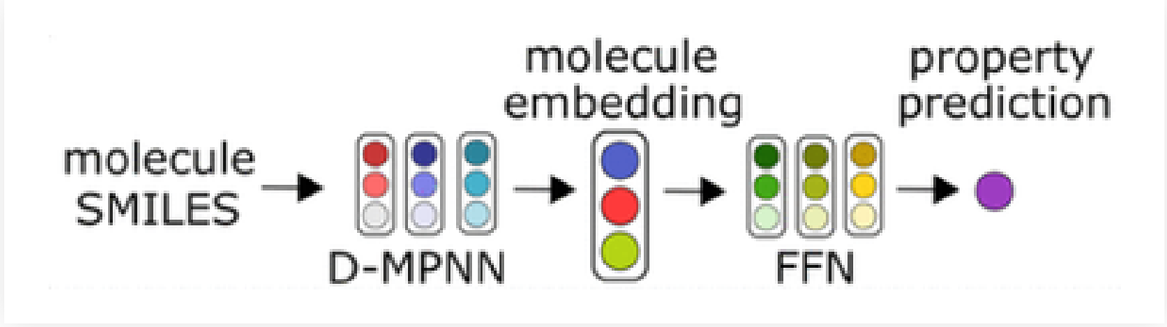


Fig 2. Chemprop treats molecules as graph structures and uses a message-passing neural network (MPNN) to learn feature representation. The MPNN is coupled with a feed-forward neural network (FFN) for property prediction. Source: Held et al., 2023

In the high-stakes race to develop much-needed drugs, such fast and accurate molecular property prediction by AI is key. Besides being utilized to discover halicin, Chemprop has been successfully used by many pharma researchers to predict drug potency, IR spectra, combination drug synergy, etc. Below are a few example workflows to show how you can reuse existing models or train new ones to predict drug properties so you can find good drug candidates with desirable ones.

Example 1: Load existing models for inferencing, e.g., solubility prediction

Chemprop relies on the PyTorch framework so one can utilize existing models loaded from checkpoint files.

Example 2: Train a new model to specific chemical libraries or properties, e.g., a toxicity classifier

Sometimes, existing models are inadequate as they may be nonexistent for a particular molecular property or may not be applicable to the chemical space of interest. Thus, it may be necessary to train a new custom model.

Example 3: Load a newly trained model registered on Databricks MLflow for inferencing, e.g., toxicity prediction

After one trains a model (Example 2), MLflow logs the model metrics and saves the model artifacts. The model can be reloaded on a notebook for prediction. It can also be registered and served so others can search and reuse it via a REST API provided by Databricks Model Serving.

Example 4: Multitask training, e.g., ADMET regression model

For a compound to be considered a good drug candidate, it must possess several desirable ADMET (absorption, distribution, metabolism, excretion, toxicity) properties such that it can be readily absorbed into the body and distributed to the target site, as well as being safely metabolized and excreted out of the body. As there may be as many as hundreds to thousands of ADMET properties to predict, it is common to do multitask training and inferencing to find good candidates possessing many of them. Multitask training is advantageous as the predicted properties are highly correlated and the joint data analysis allows knowledge gained from one task to improve another task.

Setup

Setup is straightforward as Chemprop is available as a Python package on PyPI or on GitHub. You will also need to install its dependency, rdkit-pypi

```
pip install chemprop rdkit-pypi
```

Example 1: Load existing solubility model for inference

If you already have models as PyTorch checkpoint files (*.ckpt), you can load them directly with Chemprop and use them for inferencing.

```
import torch
from lightning.pytorch import Trainer
from chemprop import data, featurizers, models

# Load model as mpnn
checkpoint_path = <ckpt_file_path>
mpnn = models.MPNN.load_from_checkpoint(checkpoint_path)
...

# Predict with the loaded mpnn
with torch.inference_mode():
    trainer = Trainer(
        logger=None,
        enable_progress_bar=True,
        accelerator="cpu",
        devices=1
    )
    test_preds = trainer.predict(mpnn, data_loader)
```

See example NB, which uses a multicomponent regressor (source: Chemprop repo) to predict if a compound would dissolve in a solvent. It expects two columns in Simplified Molecular Input Line Entry System (SMILES), a text representation of molecule structures: one for the compound to be dissolved and another representing the solvent dissolving the compound (see dataset for inferencing). The output is solubility as measured by UV-Vis spectroscopy.

COMPOUND	SOLVENT
CCCCN1C(=O)C(=C/C=C/C=C/C=C2N(CCCC)c3ccccc3N2CCCC)C(=O)N(CCCC)C1=S	ClCCl
C(=C/c1cnccn1)\c1ccc(N(c2ccccc2)c2ccc(/C=C/c3cnccn3)cc2)cc1	ClCCl
CN(C)c1ccc2c(-c3ccc(N)cc3C(=O)[O-])c3ccc(=[N+](C)C)cc-3oc2c1	O

Example 2: Train a single-task classifier

If there are no satisfactory existing models, one can train a model on specific chemical libraries or prediction properties. For example, we can train a classifier on the ClinTox database (Wu et al.), which consists of 1,491 drugs labeled if they exhibited toxicity during clinical trials (source: Huggingface). See accompanying NB.

Define model architecture

Generally, chemprop MPNN models consist of a message-passing module, an aggregation module and a final feed-forward network (FFN) module. These modules should be configured to fit the task at hand. For example, use a BinaryClassificationFFN as the output layer for binary classification and RegressionFFN for regression of continuous properties.

```
from chemprop import models, nn

mp = nn.BondMessagePassing()
agg = nn.MeanAggregation()

# If classification
ffn = nn.BinaryClassificationFFN()
metric_list = [nn.metrics.BinaryAUROC(),
               nn.metrics.BinaryAUPRC(),
               nn.metrics.BinaryAccuracy(),
               nn.metrics.BinaryF1Score()]

# If regression
# ffn = nn.RegressionFFN()
# metric_list = [nn.metrics.R2Score(),
#                nn.metrics.RMSE()]

mpnn = models.MPNN(mp, agg, ffn, batch_norm=True, metrics=metric_list)
```

Data preparation

Chemprop expects molecules to be represented as SMILES (cite) text strings. It converts SMILES into its MoleculeDatapoint class, which tracks the target property, the atoms and bonds as nodes and edges, respectively, and any additional molecular descriptors.

```
# Convert SMILES -> MoleculeData
all_data = [data.MoleculeDatapoint.from_smi(smi, y) for smi, y in
zip(smis, ys)]
```

Data splitting

As per best practices, split the data into train, validation and test datasets. Chemprop has a data module with many splitting helper functions to make this easy. However, it expects molecules as RDKit Mol objects, so we convert them accordingly as follows:

```
from chemprop import data

# MoleculeDatapoint -> RDKit Mol
mols = [d.mol for d in all_data]

train_indices, val_indices, test_indices = data.make_split_
indices(mols, "random", (0.8, 0.1, 0.1))
train_data, val_data, test_data = data.split_data_by_indices(
   all_data, train_indices, val_indices, test_indices
)
```

Once split, generate graph descriptors using an appropriate featurizer and then finally convert to a PyTorch DataLoader.

```
from chemprop import data, featurizers
# Featurization: MoleculeDatapoint -> graph descriptors
featurizer = featurizers.SimpleMoleculeMolGraphFeaturizer()

train_dset = data.MoleculeDataset(train_data[0], featurizer)
val_dset = data.MoleculeDataset(val_data[0], featurizer)
test_dset = data.MoleculeDataset(test_data[0], featurizer)

train_loader = data.build_dataloader(train_dset, num_workers=num_
workers)
val_loader = data.build_dataloader(val_dset, num_workers=num_workers)
test_loader = data.build_dataloader(test_dset, num_workers=num_workers)
```

Training

Once the above model architecture and datasets are defined, you can start training with the following few lines.

```
from lightning.pytorch import Trainer

trainer = Trainer(
   logger=False,
   enable_checkpointing=True,
   enable_progress_bar=True,
   accelerator="auto",
   max_epochs=20
   )
trainer.fit(mpnn, train_loader, val_loader)
```

Testing

Users can also test the model with the test holdout set.

```
# To get test statistics
test_stats = Trainer(logger=False).test(mpnn, test_loader)

# Inference to get prediction values
test_preds = Trainer(logger=False).predict(mpnn, test_loader)
```

Manage your trained models with MLflow

As Databricks has MLflow for model lifecycle management, it is highly recommended to log, register and serve your trained models using MLflow. Just add a couple of MLflow commands to the trainer.fit function call.

Log and register models (also autosaves models)

```
import mlflow.pytorch

mlflow.pytorch.autolog(registered_model_name=<some_model_name>)

with mlflow.start_run() as run:
   trainer.fit(mpnn, train_loader, val_loader)
mlflow.end_run()
```

Optionally, save model artifacts to a volume on Unity Catalog

You can optionally save the model files to a desired volume path on Unity Catalog, although Model Registry will have already saved the files upon registration.

```
mlflow.artifacts.download_artifacts(
   run_id=run.info.run_id,
   artifact_path="some_artifact_path",
   dst_path="some_vol_path")
```

See NB for the end-to-end execution of Example 2.

Example 3: Load model from MLflow for inferencing

If you have registered the model using MLflow, you can load it for inference with simply the following:

```
from lightning.pytorch import Trainer

model_uri = "models:/registered_model_name/model_version"
model = mlflow.pytorch.load_model(model_uri)
test_preds_reloaded = Trainer(logger=False).predict(model, drugbank_
loader)
```

To get the model_uri, check out these options.

This example NB shows how the model trained in Example 2 was loaded from MLflow and used to predict the clinical toxicity using DrugBank, a database of over 2,000 FDA-approved small molecule drugs (source: doi.org/10.5281/zenodo.10372418).

Example 4: Train multitask ADMET regression model

For a compound to be considered a good drug candidate, it must possess several desirable ADMET properties such as bioavailability, high potency and low toxicity. In this example, we trained a multitask regression model on 10 continuous ADMET properties from the Therapeutics Data Commons simultaneously (doi.org/10.5281/zenodo.10372418). It is advantageous to do multitask training as the predicted properties are highly correlated and the joint data analysis facilitates knowledge gained from one task to improve another task.

Table 1: Sample training data with 10 continuous ADMET properties for multitask regression

SMILES	C=C[C@H]1CN2CC[C@H]1C[C@@H]2[C@@H](O)c1ccnc2ccc(OC)cc12	CC(=O)Nc1ccc(O)cc1	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1
Caco2_Wang	-4.6900001	-4.4400001	-4.4699998
Clearance_Hepatocyte_AZ	6.17	6.31	7.41
Clearance_Microsome_AZ	null	3	18.62
Half_Life_Obach	6.6	2.5	null
HydrationFreeEnergy_FreeSolv	null	null	null
LD50_Zhu	null	1.799	null
Lipophilicity_AstraZeneca	2.21	0.25	3.35
PPBR_AZ	85.48	26.64	95.82
Solubility_AqSolDB	-2.81214297	-1.033323213	null
VDss_Lombardo	null	1	0.77

The code is similar to single-task training (Example 2), except that the final FFN has to accommodate the 10 targets that are co-trained. Thus, we define the FFN with 10 tasks as follows:

```
ffn = nn.RegressionFFN(n_tasks=10)
```

Once trained, the multitask regressor can be used to predict the 10 ADMET properties of DrugBank loaded for inferencing in Example 3.

See these links for the end-to-end execution for multitask training and multitask inferencing.

Conclusions

This blog provides a quickstart guide for how to use Chemprop to load existing models to train new models and perform a variety of single-/multitask molecular property predictions. To learn more, check out the official tutorials from Chemprop.

CHAPTER 7:

Applying Image Classification With PyTorch Lightning on Databricks

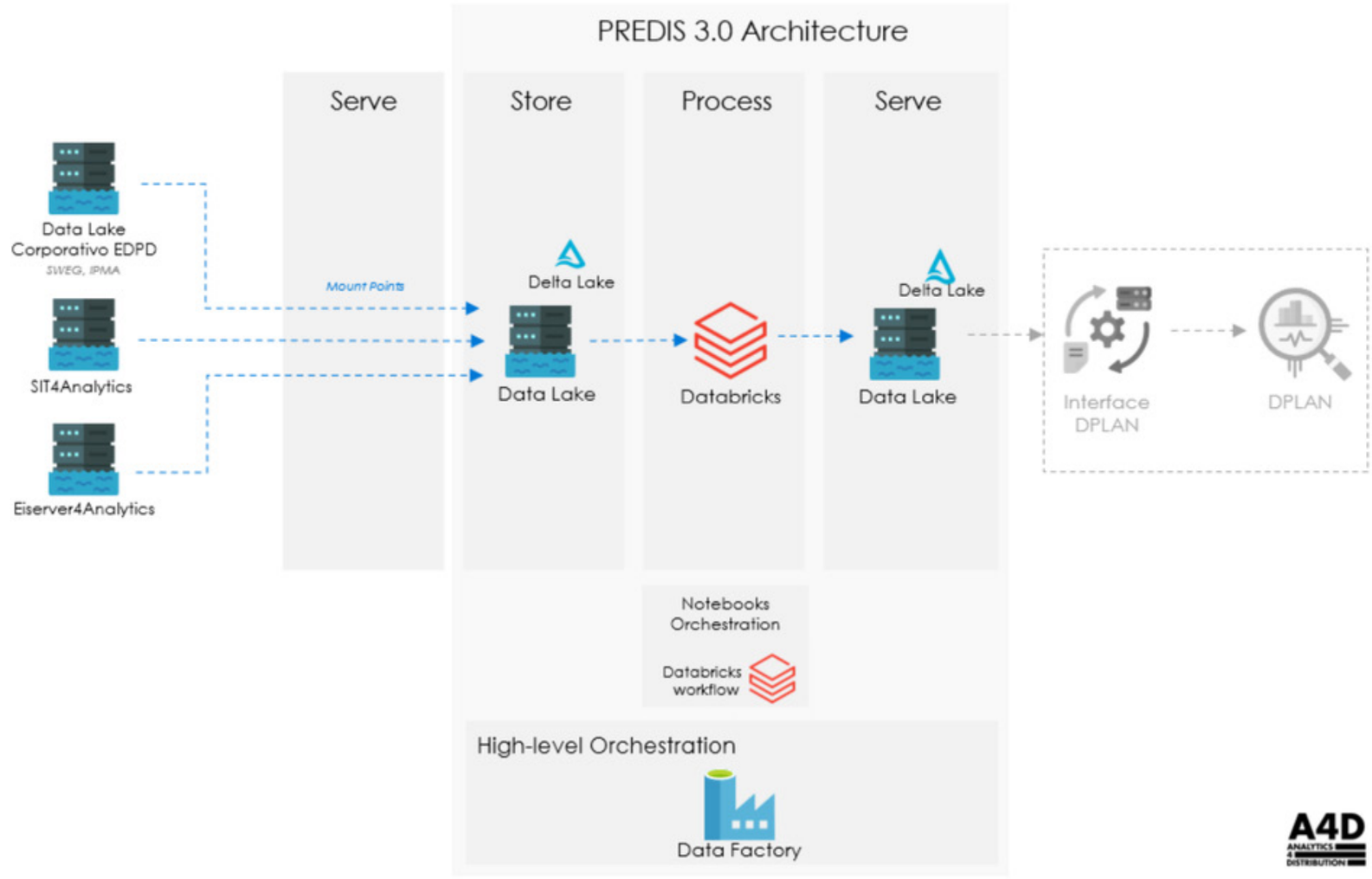
Traditionally, power grids have been sized with large safety margins to consider low-probability events. Thus, there can be limits imposed on generation even when the low-probability events do not occur. Generation and load forecasting coupled with power-flow analysis will allow E-REDES to estimate the power flowing in each line of the HV and MV grid. Thus, E-REDES can allow for increased generation in the grid using the existing infrastructure. It is possible that the grid generation hosting capacity can be increased by 20%, or even more, depending on the particular case.

PREDIS is a big data time series forecasting project whose goal is to predict 200K load diagrams, each with a 15-minute granularity, and daily for all medium- and high-voltage installations of the Portuguese electrical grid.

To tackle this ambitious task, the PREDIS daily inference pipeline relies on an ensemble of three state-of-the-art forecasting models — Elastic Net, LightGBM and Prophet — together with a baseline model that outputs the previous day's load data. Each day, the individual model whose inference on the previous day over a given time series performed better (with respect to the MAE metric) is chosen to infer the next three days.

Both training and inference pipelines are heavily data-dependent. The former used two years of historical data (comprising 14.5B records), while the latter uses every day, and for each individual time series, a year's worth of historical data to fit the series and infer it. This compute-intensive workload is leveraged exclusively by Databricks and Spark.

Architecture and tech stack



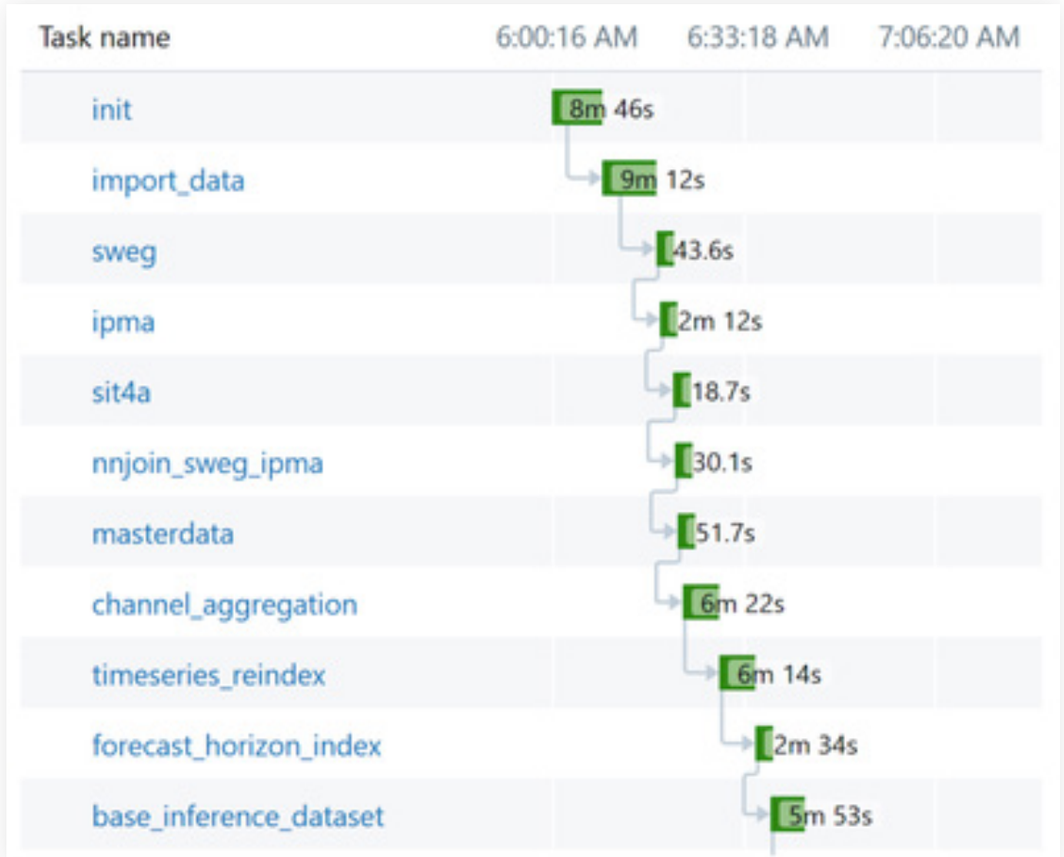
Here's a summary of our tech stack:

- **Cloud provider:** Azure
- **Data storage:** Corporate and project data are stored in a dedicated data lake with Delta tables
- **Development environment:** Fully developed in Databricks Notebooks using PySpark, Python and vectorized UDFs
- **Notebooks orchestration:** Both training and inference pipelines are orchestrated through Lakeflow Jobs and running in job clusters
- **Resource orchestration:** High-level orchestration through Azure Data Factory triggering Lakeflow Jobs via API
- **Forecast access:** Forecasts written to an Oracle database and accessed by the network planning and optimization E-REDES system
- **Data loading:** Outputs are written into an Oracle database through Azure Data Factory
- **DevOps:** CI/CD pipelines managed with Azure DevOps. Model training is performed in the development environment, while inference runs daily in the production environment.

Data sources

- **Load diagrams**
  This main data source provides meter data from all high- and medium-voltage installations across the Portuguese electrical grid. Every day, PREDIS ingests a staggering 60 million new records. The input dataset encompasses 96 measurements per asset for 100,000 installations and six types of energy consumption, comprising the core of our load forecasting efforts.
- **Grid technical information**
  This data source provides essential registry and geographic information for all electrical grid assets and installations.
- **Weather forecasts**
  The IPMA (Portuguese Institute for Sea and Atmosphere) source supplies weather forecasts up to three days in advance, which are incorporated as exogenous variables in our models. These weather forecasts are pivotal for creating external factors that influence energy demand, such as temperature fluctuations and precipitation, thereby enhancing the accuracy of our predictions.

ETL workflow



Our ETL (extract, transform, load) comprises several Databricks notebooks, each playing a specific role in transforming the raw data. Below is an overview of the data transformations that form the backbone of PREDIS.

- **Data ingestion and initial processing**
  All data sources are first imported into the Bronze database (notebook import_data). Each source undergoes an individual processing before combining all sources in a single master data table (this time persisted in the Silver database).
- **Weather forecast integration**
  To incorporate weather data into our forecasts, we perform a nearest neighbor join (notebook nnjoin_sweg_ipma) to determine the closest weather forecast grid point for each installation. This step ensures that weather data is accurately aligned with the specific locations of our assets.
- **Master data table**
  A master data table is created to maintain a comprehensive record of all installation keys and static attributes. This table serves as a reference for linking dynamic data with static installation information.
- **Data aggregation**
  The raw meter data, which is reported in six separate channels, is aggregated into two main channels: active and reactive energy. This aggregation simplifies the dataset and focuses the forecasting models on the data most relevant to the business.

- **Handling missing data**
  Data points missing due to communication failures or other issues are addressed by reindexing the time series (notebook timeseries_reindexed). This process involves adding missing time steps according to a fixed start and end date, ensuring continuity in the time series data.
- **Inference dataset creation**
  Finally, we compile the inference dataset by joining all processed data sources, including weather forecast parameters required for accurate predictions (notebooks forecast_horizon_index and base_inference_dataset). This dataset forms the basis for generating forecasts and is used to train and validate the forecasting models.

Scalability

The ETL and preprocessing pipeline is scalable by design. The process manages huge amounts of data by leveraging Databricks and Apache Spark with pandas UDFs for distributed data processing.

- **Training pipeline:** Processed two years of historical data, resulting in a dataset with 14.5 billion records
- **Inference pipeline:** Processes one year of historical data every day to fit the models and generate forecasts

Time series forecasting

For each load diagram, we daily fit three local time series models, namely:

- **Elastic Net Regression:** This model employs an autoregressive approach which assumes that the current value of a time series is influenced by its past values. Elastic Net Regression enhances the basic linear regression model by incorporating regularization to manage overfitting and model complexity. Specifically, L2 regularization increases the model's resilience to multicollinearity, while L1 regularization aids in excluding irrelevant features. To extend forecasts beyond ***t+1***, a recursive strategy is employed, where the model's previous forecast is used as an input feature to predict subsequent time steps.
  - Combines the best of both worlds: Elastic Net merges the strengths of Ridge and Lasso regression techniques. It helps in picking out important features like Lasso and stabilizes the model with regularization like Ridge.
  - Handles multicollinearity: Elastic Net is great at dealing with multicollinearity, which means it can manage situations where features are highly correlated, thanks to its Ridge regularization
  - Selects key features: If you have lots of predictors and suspect many might be irrelevant, Elastic Net can help select the most important ones thanks to the Lasso regularization

- **LightGBM:** This gradient boosting tree-based model includes built-in feature importance and constructs decision trees sequentially. Each tree is designed to correct the errors of its predecessor, allowing the model to effectively capture seasonality and complex patterns in time series data. Similar to Elastic Net Regression, LightGBM (Light Gradient Boosting Machine) extends forecasts using a recursive strategy.
  - Handles complex relationships: LightGBM excels at capturing complex, nonlinear patterns in your data that simpler models might miss
  - Efficient and fast: It's designed to be quick and efficient with memory, making it ideal for large datasets
  - High accuracy: LightGBM often outperforms traditional machine learning models in terms of accuracy due to its ability to capture intricate patterns
  - Seasonality and trends: Although not specifically for time series, LightGBM can incorporate time-based features (like month, day, hour) to help capture seasonal and trend patterns
- **Prophet:** Developed by Facebook, Prophet is a forecasting model that identifies seasonal patterns in time series data. Known for its intuitive approach, Prophet typically yields good results with minimal tuning and effort.
  - Built for time series: Prophet, developed by Facebook, is specifically designed for forecasting time series data. It handles seasonality, holidays and trend changes effectively.
  - User-friendly: It is easy to use and allows for intuitive parameter tuning, making it accessible even to those without deep expertise in time series analysis
  - Seasonality: Prophet can handle multiple seasonalities (daily, weekly, yearly) and even custom seasonal patterns, leveraging its built-in capabilities for handling various seasonal effects and holidays
  - Trends and anomalies: Prophet can detect and model long-term trends and identify anomalies or change points in your data

In all three models, weather forecast variables and holidays are incorporated as exogenous variables to enhance the accuracy of the predictions. This approach ensures you can capture a wide range of patterns and trends in your time series data, leading to more accurate and robust forecasts.

Cross-validation

A sliding window approach was employed for cross-validation. The two-year training dataset was evenly split into seven segments, each based on a 60-day interval. The models were trained using the training set to predict the validation set up to five days ahead, and error metrics were estimated. The average of all metric scores across these folds provided the final validation score, which was used to determine the optimal hyperparameters.

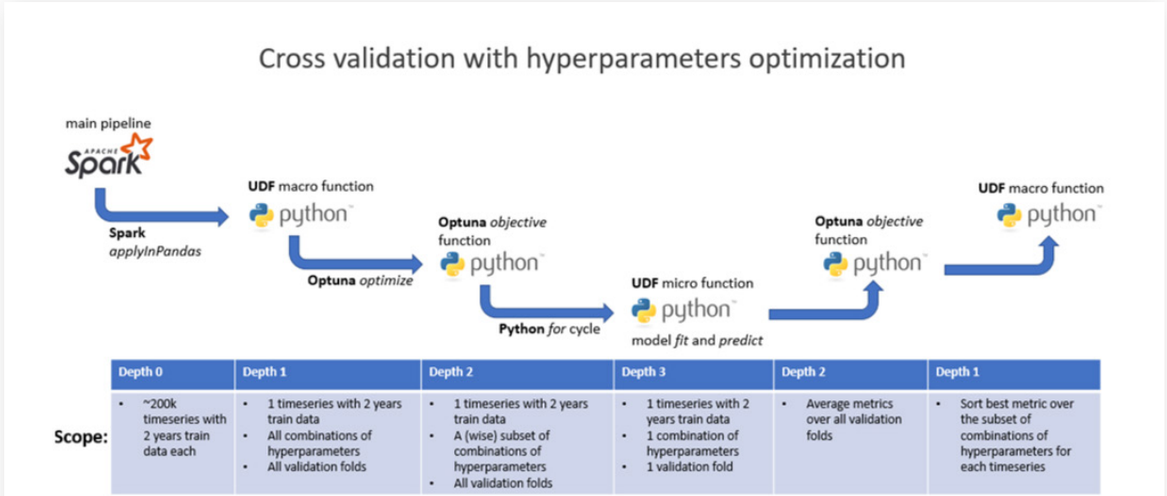
Given the impracticality of an exhaustive hyperparameter tuning strategy for this big data problem, we adopted a Bayesian optimization approach implemented through the Optuna library, instead of a brute-force method like grid search. Optuna leverages past experiments to suggest new hyperparameters, aiming to find the optimal solution by minimizing an error metric.

The training process was optimized by conducting 20 Optuna tuning experiments for both Prophet and LightGBM models. Due to the faster adjustment time of Elastic Net Regression, it was trained with 28 tuning experiments per time series.

The metrics used include:

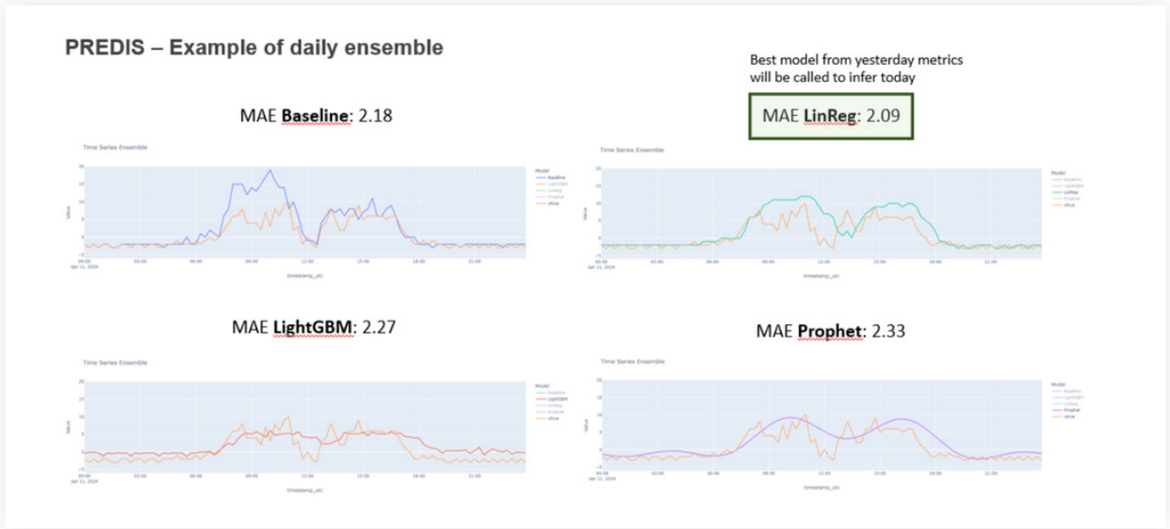
- Mean Squared Error (MSE): Used for minimizing error during optimization
- Normalized Mean Absolute Error (NMAE) and Normalized Mean Squared Error (NMSE): Used for reporting metrics to business stakeholders. The installed power of each installation was used to normalize these metrics.

Considering the large-scale time series inference dataset, we used pandas UDFs to parallelize the training across the entire universe of time series. This process took approximately six days per model for the 200K time series. A key optimization tip from Databricks was to turn off Adaptive Query Execution (AQE) and manually repartition by the distinct number of time series.



Inference

Based on the optimized hyperparameters for each time series model, the inference pipeline includes the ETL processes described previously, followed by model inference. Given the substantial volume of data, we once again used pandas UDFs to evenly distribute the inference workload. The pipeline incorporates three machine learning models along with a baseline model that predicts the previous day's values. The final model chosen for inference each day is the one that performed best on the previous day, as exemplified below.



While the Linear Regression model performed better in this specific instance, all models are generally used for inference. As anticipated, the inference results were slightly less accurate compared to the training phase. This discrepancy arises because the models were trained with data from 2022 and 2023, and the distribution of each time series could have changed in the meantime. To maintain model accuracy, we plan to retrain the models annually to update the optimized hyperparameters.

The inference process takes approximately three hours to execute using a dedicated cluster with 40 nodes.

Test dataset

A daily metrics pipeline runs after the inference pipeline, in a separate Databricks workflow with lighter compute infrastructure. The objective is to calculate daily error metrics for all time series and all models by comparing the real measurements with the past forecasted values. In this case only MAE (mean absolute error) and MSE (mean normalized error) are recorded for up to two years of history. Later, these values are used to report the official PREDIS test metrics, by normalizing each metric by the installation's nominal power and creating different aggregations — for example, "Normalized RMSE by Model, Installation and Channel."

This metrics history will be used to create a "Model Monitoring" dashboard where business users can inspect the quality of the forecasts at both an individual and aggregated level.

Snippets of code

```
def prophet_hyperparameter_optimization(df, df_folds):
   # df: Pandas dataframe with a full timeseries
   # df_folds: dataframe with crossvalidation folds to run (start_date
and end_date of each fold)

   # save key values
   key = df["key"].iloc[0]

   # create timeseries, set time index, sort index
   df = (
       df[["timestamp_utc", "value", *exog_columns]]
       .set_index("timestamp_utc")
       .sort_index()
   )
   df.index.freq = "15min"

   # use Optuna library to find the combination of hyperparameters that
minimizes the validation metric (MSE)
   study = optuna.create_study(
       direction="minimize",
       sampler=optuna.samplers.TPESampler(
           n_startup_trials=n_startup_trials, multivariate=True
       ),
   )

   # optuna optimize ()
   study.optimize(
       lambda trial: prophet_crossvalidation(trial, df, df_folds), n_
trials=n_trials
   )

 # get best metrics
   study_scores = {**study.best_trial.user_attrs}
   study_scores["key"] = key

   # add hyperparameters
   study_scores["hyperparameters"] = json.dumps(study.best_params)

   # add training time of best trial
   study_scores["duration"] = (
       study.best_trial.datetime_complete - study.best_trial.datetime_
start
   ).seconds

   # convert to pandas
   study_scores = pd.DataFrame([study_scores])

   return study_scores[
       ["key", "hyperparameters", "mean_score_mae", "mean_score_mse",
"duration"]
   ]
```

Figure 1. Example of a Python function that performs Bayesian hyperparameter optimization with Optuna.

```
# disable spark AQE config, to avoid incompatibility with UDFs
# AQE might overwrite the repartition operation defined below
spark.conf.set("spark.sql.adaptive.enabled", "false")

# repartition by distinct number of timeseries and key columns
# groupby key columns and use applyInPandas to execute the
crossvalidation UDF
# the "df_parameters" is a dictionary with all validation sets to run
# this means each core of each worker/executor will run its own task/
crossvalidation
key_columns = ["key"]
df = (
   df.repartition(df.select(*key_columns).distinct().count(), *key_
columns)
   .groupBy(*key_columns)
   .applyInPandas(
       lambda df: prophet_hyperparameter_optimization(df, df_
parameters), schema
   )
)
```

Figure 2. Example of distributed training using pandas UDF and manually repartitioning by distinct number of time series keys. Adaptive Query Execution (AQE) must be disabled to ensure that the repartition takes effect.

Final thoughts and future work

The PREDIS project represents a significant achievement for E-REDES in time series forecasting for energy demand and supply.

Achievements

1. **Advanced forecasting capabilities:** Implementing Elastic Net Regression, LightGBM and Prophet models alongside a baseline model has enabled accurate daily forecasts for approximately 200K load diagrams, providing precise and actionable predictions for medium- and high-voltage installations in the Portuguese grid.
2. **Scalable and efficient pipeline design:** Our ETL and preprocessing pipeline, developed using Databricks and Apache Spark with pandas UDFs, has effectively managed large-scale data demands. Bayesian optimization with Optuna has enhanced model performance in big data environments.
3. **Effective inference process:** A high-performance inference pipeline, run on a 40-node cluster, enables daily forecasts and model selection, demonstrating the capacity to handle large datasets and generate timely predictions.

Lessons learned

1. **Model selection and ensemble methods:** The importance of selecting the most effective model for each time series has been emphasized. Future work will refine ensemble methods and integrate new models to enhance forecast accuracy.
2. **Adaptation to data changes:** Regular retraining is crucial for maintaining high forecast accuracy, given the observed degradation in model performance over time. Annual updates to the models are planned to adapt to evolving data distributions.
3. **Optimization strategies:** Effective use of pandas UDFs and manual repartitioning has improved the efficiency of cross-validation and inference processes. Future efforts will explore further optimization techniques to streamline these processes.

Future work

- **Exploration of global models:** Investigating global models as alternatives to current local models could improve forecasting accuracy
- **Development of automated model selection mechanisms:** Creating automated model selection methodology based on historical performance patterns could enhance the efficiency of the inference pipeline
- **Expansion of model ensemble techniques:** Adding new models to the existing ensemble to target different data patterns and forecasting challenges may yield more robust and accurate solutions
- **Enhancement of hyperparameter optimization:** Continued refinement of hyperparameter optimization strategies will further improve model performance and forecasting accuracy
- **MLflow integration with Optuna:** Record and track all Optuna trials during future retrainings with MLflow

In conclusion, the PREDIS project has successfully demonstrated the application of state-of-the-art forecasting models and advanced data processing techniques. The insights gained pave the way for future innovations in time series forecasting and energy management for E-REDES.

About E-REDES

E-REDES is a Distribution System Operator (DSO) supplying electricity to all connected consumers across Portugal.

Mission: supply electricity to all consumers, ensuring quality, security and efficiency while promoting a sustainable grid development that supports the energy transition and is able to provide, in a neutral way, services to the market agents.

- One high-/medium-voltage concession granted by the government
- 278 low-voltage concessions granted by municipalities

CHAPTER 8:

Processing Geospatial Data at Scale With Databricks

By **Nima Razavi** and **Michael Johns**

The evolution and convergence of technology has fueled a vibrant marketplace for timely and accurate geospatial data. Every day, billions of handheld and IoT devices along with thousands of airborne and satellite remote sensing platforms generate hundreds of exabytes of location-aware data. This boom of geospatial big data combined with advancements in machine learning is enabling organizations across industries to build new products and capabilities.

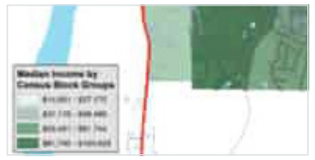
FRAUD AND ABUSE

Detect patterns of fraud and collusion (e.g., claims fraud, credit card fraud)

RETAIL

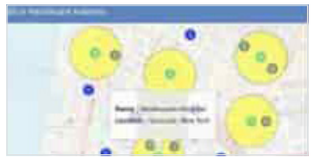
Site selection, urban planning, foot traffic analysis

FINANCIAL SERVICES



Economic distribution, loan risk analysis, predicting sales at retail, investments

HEALTHCARE



Identifying disease epicenters, environmental impact on health, planning care

DISASTER RECOVERY

Flood surveys, earthquake mapping, response planning

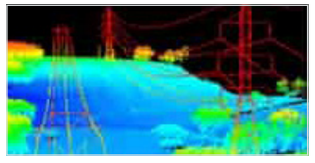
DEFENSE AND INTEL

Reconnaissance, threat detection, damage assessment

INFRASTRUCTURE

Transportation planning, agriculture management, housing development

ENERGY



Climate change analysis, energy asset inspection, oil discovery

Maps leveraging geospatial data are used widely across industries, spanning multiple use cases, including disaster recovery, defense and intel, infrastructure and health services.

For example, numerous companies provide localized drone-based services such as mapping and site inspection (reference Developing for the Intelligent Cloud and Intelligent Edge). Another rapidly growing industry for geospatial data is autonomous vehicles. Startups and established companies alike are amassing large corpuses of highly contextualized geodata from vehicle sensors to deliver the next innovation in self-driving cars (reference Databricks fuels wejo's ambition to create a mobility data ecosystem). Retailers and government agencies are also looking to make use of their geospatial data. For example, foot-traffic analysis (reference Building Foot-Traffic Insights Data Set) can help determine the best location to open a new store or, in the public sector, improve urban planning. Despite all these investments in geospatial data, a number of challenges exist.

Challenges analyzing geospatial at scale

The first challenge involves dealing with scale in streaming and batch applications. The sheer proliferation of geospatial data and the SLAs required by applications overwhelms traditional storage and processing systems. Customer data has been spilling out of existing vertically scaled geodatabases into data lakes for many years now due to pressures such as data volume, velocity, storage cost and strict schema-on-write enforcement. While enterprises have invested in geospatial data, few have the proper technology architecture to prepare these large, complex data sets for downstream analytics. Further, given that scaled data is often required for advanced use cases, the majority of AI-driven initiatives are failing to make it from pilot to production.

Compatibility with various spatial formats poses the second challenge. There are many different specialized geospatial formats established over many decades as well as incidental data sources in which location information may be harvested:

- Vector formats such as GeoJSON, KML, shapefile and WKT
- Raster formats such as ESRI Grid, GeoTIFF, JPEG 2000 and NITF
- Navigational standards such as used by AIS and GPS devices
- Geodatabases accessible via JDBC/ODBC connections such as PostgreSQL/PostGIS
- Remote sensor formats from hyperspectral, multispectral, lidar and radar platforms
- OGC web standards such as WCS, WFS, WMS and WMTS
- Geotagged logs, pictures, videos and social media
- Unstructured data with location references

In this blog post, we give an overview of general approaches to deal with the two main challenges listed above using the Databricks Unified Data Analytics Platform. This is the first part of a series of blog posts on working with large volumes of geospatial data.

Scaling geospatial workloads with Databricks

Databricks offers a unified data analytics platform for big data analytics and machine learning used by thousands of customers worldwide. It is powered by Apache Spark™, Delta Lake and MLflow with a wide ecosystem of third-party and available library integrations. Databricks UDAP delivers enterprise-grade security, support, reliability and performance at scale for production workloads. Geospatial workloads are typically complex, and there is no one library fitting all use cases. While Apache Spark does not offer geospatial Data Types natively, the open source community as well as enterprises have directed much effort to develop spatial libraries, resulting in a sea of options from which to choose.

There are generally three patterns for scaling geospatial operations such as spatial joins or nearest neighbors:

1. Using purpose-built libraries that extend Apache Spark for geospatial analytics. GeoSpark, GeoMesa, GeoTrellis and RasterFrames are a few of such libraries used by our customers. These frameworks often offer multiple language bindings and have much better scaling and performance than non-formalized approaches, but can also come with a learning curve.
2. Wrapping single-node libraries such as GeoPandas, Geospatial Data Abstraction Library (GDAL) or Java Topology Suite (JTS) in ad hoc user-defined functions (UDFs) for processing in a distributed fashion with Spark DataFrames. This is the simplest approach for scaling existing workloads without much code rewrite; however, it can introduce performance drawbacks as it is more lift-and-shift in nature.
3. Indexing the data with grid systems and leveraging the generated index to perform spatial operations is a common approach for dealing with very large-scale or computationally restricted workloads. S2, GeoHex and Uber's H3 are examples of such grid systems. Grids approximate geo features such as polygons or points with a fixed set of identifiable cells, thus avoiding expensive geospatial operations altogether, and thus offer much better scaling behavior. Implementers can decide between grids fixed to a single accuracy that can be somewhat lossy yet more performant or grids with multiple accuracies that can be less performant but mitigate against lossines.

The following examples are generally oriented around a New York City taxi pickup/drop-off data set found here. NYC Taxi Zone data with geometries will also be used as the set of polygons. This data contains polygons for the five boroughs of NYC as well the neighborhoods. This notebook will walk you through preparations and cleanings done to convert the initial CSV files into Delta Lake tables as a reliable and performant data source.

Our base DataFrame is the taxi pickup/drop-off data read from a Delta Lake Table using Databricks.

```
%scala
val dfRaw = spark.read.format("delta").load("/ml/blogs/geospatial/
delta/nyc-green")
display(dfRaw) // showing first 10 columns
```

vendor_id	pickup_datetime	dropoff_datetime	store_and_forward	rate_code_id	pickup_longitude	pickup_latitude	dropoff_longitude	dropoff_latitude	passener_count
2	2017-09-30 23:48:04	2017-09-30 23:57:43	N	1	82	7	2	1.89	9
2	2017-09-30 23:50:24	2017-09-30 23:55:30	N	1	25	181	6	1.26	6
2	2017-09-30 23:28:29	2017-09-30 23:37:29	N	1	41	159	1	2.28	9
2	2017-09-30 23:46:44	2017-09-30 23:54:59	N	1	42	41	1	1.09	7
2	2017-09-30	2017-09-30 23:31:49	N	1	33	189	1	2.35	10

Showing the first 1000 rows.

Figure 1: Geospatial data read from a Delta Lake table using Databricks

Geospatial operations using geospatial libraries for Apache Spark

Over the last few years, several libraries have been developed to extend the capabilities of Apache Spark for geospatial analysis. These frameworks bear the brunt of registering commonly applied user-defined types (UDT) and functions (UDF) in a consistent manner, lifting the burden otherwise placed on users and teams to write ad hoc spatial logic. Please note that in this blog post, we use several different spatial frameworks chosen to highlight various capabilities. We understand that other frameworks exist beyond those highlighted, which you might also want to use with Databricks to process your spatial workloads.

Earlier, we loaded our base data into a DataFrame. Now we need to turn the latitude/longitude attributes into point geometries. To accomplish this, we will use UDFs to perform operations on DataFrames in a distributed fashion. Please refer to the provided notebooks at the end of the blog for details on adding these frameworks to a cluster and the initialization calls to register UDFs and UDTs. For starters, we have added GeoMesa to our cluster, a framework especially adept at handling vector data. For ingestion, we are mainly leveraging its integration of JTS with Spark SQL, which allows us to easily convert to and use registered JTS geometry classes. We will be using the function st_makePoint that, given a latitude and longitude, create a Point geometry object. Since the function is a UDF, we can apply it to columns directly.

```
%scala
val df = dfRaw
 .withColumn("pickup_point", st_makePoint(col("pickup_longitude"),
col("pickup_latitude")))
 .withColumn("dropoff_point", st_makePoint(col("dropoff_
longitude"),col("dropoff_latitude")))
display(df.select("dropoff_point","dropoff_datetime"))
```

(2) Spark Jobs

dropoff_point	dropoff_datetime
POINT (-73.98411560058594 40.695980072021484)	2016-04-01 00:05:53
POINT (-73.8504409790039 40.724143981933594)	2016-04-01 00:05:55

Showing the first 1000 rows.

Figure 2: Using UDFs to perform operations on DataFrames in a distributed fashion to turn geospatial data latitude/longitude attributes into point geometries.

We can also perform distributed spatial joins, in this case using GeoMesa's provided st_contains UDF to produce the resulting join of all polygons against pickup points.

```
%scala
val joinedDF = wktDF.join(df, st_contains($"the_geom", $"pickup_point")
display(joinedDF.select("zone","borough","pickup_point","pickup_
datetime"))
```

(2) Spark Jobs

zone	borough	pickup_point	pickup_datetime
Fort Greene	Brooklyn	POINT (-73.98096466064453 40.689029693603516)	2016-06-09 10:35:08
Crown Heights North	Brooklyn	POINT (-73.95674896240234 40.67413330078125)	2016-06-09 10:42:15
Brooklyn Heights	Brooklyn	POINT (-73.9929428100586 40.69749069213867)	2016-06-09 10:47:38
Brooklyn Heights	Brooklyn	POINT (-73.99117279052734 40.6959114074707)	2016-06-09 10:46:09
Williamsburg (South Side)	Brooklyn	POINT (-73.96204376220703 40.70991516113281)	2016-06-09 10:06:12
East Harlem North	Manhattan	POINT (-73.93933868408203 40.80525207519531)	2016-06-09 10:58:19
Steinway	Queens	POINT (-73.9175796508789 40.76995468396484)	2016-06-09 10:45:41
Morningside Heights	Manhattan	POINT (-73.96385192871094 40.80808639526367)	2016-06-09 10:36:34

Showing the first 1000 rows.

Figure 3: Using GeoMesa's provided st_contains UDF, for example, to produce the resulting join of all polygons against pickup points

Wrapping single-node libraries in UDFs

In addition to using purpose-built distributed spatial frameworks, existing single-node libraries can also be wrapped in ad hoc UDFs for performing geospatial operations on DataFrames in a distributed fashion. This pattern is available to all Spark language bindings — Scala, Java, Python, R and SQL — and is a simple approach for leveraging existing workloads with minimal code changes. To demonstrate a single-node example, let's load NYC borough data and define UDF find_borough(...) for point-in-polygon operation to assign each GPS location to a borough using geopandas. This could also have been accomplished with a vectorized UDF for even better performance

```
%python
# read the boroughs polygons with geopandas
gdf = gdp.read_file("/dbfs/ml/blogs/geospatial/nyc_boroughs.geojson")

b_gdf = sc.broadcast(gdf) # broadcast the geopandas dataframe to all
nodes of the cluster
def find_borough(latitude,longitude):
  mgdf = b_gdf.value.apply(lambda x: x["boro_name"] if x["geometry"].
intersects(Point(longitude, latitude))
  idx = mgdf.first_valid_index()
  return mgdf.loc[idx] if idx is not None else None

find_borough_udf = udf(find_borough, StringType())
```

Now we can apply the UDF to add a column to our Spark DataFrame, which assigns a borough name to each pickup point.

```
%python
# read the coordinates from delta
df = spark.read.format("delta").load("/ml/blogs/geospatial/delta/nyc-green")
df_with_boroughs = df.withColumn("pickup_borough", find_borough_udf(col("pickup_latitude"),col(pickup_longitude)))
display(df_with_boroughs.select(
  "pickup_datetime","pickup_latitude","pickup_longitude","pickup_borough"))
```

▸ (2) Spark Jobs

pickup_datetime	pickup_latitude	pickup_longitude	pickup_borough
2016-04-01 00:06:39	40.718135833740234	-73.95951080322266	Manhattan
2016-04-01 00:06:28	40.86066818237305	-73.88964080810547	Manhattan
2016-04-01 00:07:25	40.73863983154297	-73.88591766357422	Manhattan
2016-04-01 00:09:44	40.69947814941406	-73.92366790771484	Manhattan
2016-04-01 00:16:02	40.691192626953125	-73.9872055053711	Manhattan
2016-04-01 00:14:52	40.761085510253906	-73.92341613769531	Manhattan
2016-04-01 00:11:00	40.686092376708984	-73.97399139404297	Manhattan
2016-04-01 00:17:17	40.79181671142578	-73.944580078125	Manhattan
2016-04-01 00:23:22	40.80267660522461	-73.95506134476562	Manhattan

Showing the first 1000 rows.

Figure 4: The result of a single-node example, where GeoPandas is used to assign each GPS location to an NYC borough

Grid systems for spatial indexing

Geospatial operations are inherently computationally expensive. Point-in-polygon, spatial joins, nearest neighbor or snapping to routes all involve complex operations. By indexing with grid systems, the aim is to avoid geospatial operations altogether. This approach leads to the most scalable implementations with the caveat of approximate operations. Here is a brief example with H3.

Scaling spatial operations with H3 is essentially a two-step process. The first step is to compute an H3 index for each feature (points, polygons, ...) defined as UDF geoToH3(...). The second step is to use these indices for spatial operations such as spatial join (point-in-polygon, k-nearest neighbors, etc.), in this case defined as UDF multiPolygonToH3(...).

```
%scala
import com.uber.h3core.H3Core
import com.uber.h3core.util.GeoCoord
import scala.collection.JavaConversions._
import scala.collection.JavaConverters._

object H3 extends Serializable {
  val instance = H3Core.newInstance()
}

val geoToH3 = udf{ (latitude: Double, longitude: Double, resolution:
Int) =>
  H3.instance.geoToH3(latitude, longitude, resolution)
}

val polygonToH3 = udf{ (geometry: Geometry, resolution: Int) =>
  var points: List[GeoCoord] = List()
  var holes: List[java.util.List[GeoCoord]] = List()
  if (geometry.getGeometryType == "Polygon") {
    points = List(
      geometry
        .getCoordinates()
        .toList
        .map(coord => new GeoCoord(coord.y, coord.x)): _*)
  }
  H3.instance.polyfill(points, holes.asJava, resolution).toList
}
```

```
val multiPolygonToH3 = udf{ (geometry: Geometry, resolution: Int) =>
  var points: List[GeoCoord] = List()
  var holes: List[java.util.List[GeoCoord]] = List()
  if (geometry.getGeometryType == "MultiPolygon") {
    val numGeometries = geometry.getNumGeometries()
    if (numGeometries > 0) {
      points = List(
        geometry
          .getGeometryN(0)
          .getCoordinates()
          .toList
          .map(coord => new GeoCoord(coord.y, coord.x)): _*)
    }
    if (numGeometries > 1) {
      holes = (1 to (numGeometries - 1)).toList.map(n => {
        List(
          geometry
            .getGeometryN(n)
            .getCoordinates()
            .toList
            .map(coord => new GeoCoord(coord.y, coord.x)): _*).asJava
      })
    }
  }
  H3.instance.polyfill(points, holes.asJava, resolution).toList
}
```

We can now apply these two UDFs to the NYC taxi data as well as the set of borough polygons to generate the H3 index.

```
%scala
val res = 7 //the resolution of the H3 index, 1.2km
val dfH3 = df.withColumn(
  "h3index",
  geoToH3(col("pickup_latitude"), col("pickup_longitude"), lit(res))
)
val wktDFH3 = wktDF
  .withColumn("h3index", multiPolygonToH3(col("the_geom"), lit(res)))
  .withColumn("h3index", explode($"h3index"))
```

Given a set of lat/lon points and a set of polygon geometries, it is now possible to perform the spatial join using h3index field as the join condition. These assignments can be used to aggregate the number of points that fall within each polygon, for instance. There are usually millions or billions of points that have to be matched to thousands or millions of polygons, which necessitates a scalable approach. There are other techniques not covered in this blog that can be used for indexing in support of spatial operations when an approximation is insufficient.

```
%scala
val dfWithBoroughH3 = dfH3.join(wktDFH3,"h3index")

display(df_with_borough_h3.select("zone","borough","pickup_
point","pickup_datetime","h3index"))
```

▸ (1) Spark Jobs

zone	borough	pickup_point	pickup_datetime	h3index
Morningside Heights	Manhattan	POINT (-73.95296478271484 40.80758285522461)	2016-06-09 10:14:34	613229523000885247
Central Harlem	Manhattan	POINT (-73.94908905029297 40.80293655395508)	2016-06-09 10:04:08	613229523028148223
Brooklyn Heights	Brooklyn	POINT (-73.99422454833984 40.69488525390625)	2016-06-09 10:52:24	613229551411003391
Van Nest/Morris Park	Bronx	POINT (-73.84475708007812 40.847774505615234)	2016-06-09 10:23:52	613229520937287679
Astoria	Queens	POINT (-73.9139633178711 40.76524353027344)	2016-06-09 10:25:38	613229524726841343
Morningside Heights	Manhattan	POINT (-73.95944213867188 40.80912399291992)	2016-06-09 10:42:56	613229523000885247
Park Slope	Brooklyn	POINT (-73.97588348388672 40.67397689819336)	2016-06-09 10:53:01	613229552669294591
East Harlem North	Manhattan	POINT (-73.95088058740234 40.79750061035156)	2016-06-09 10:02:37	613229523015565311

Showing the first 1000 rows.

Figure 5: DataFrame table representing the spatial join of a set of lat/lon points and polygon geometries, using a specific field as the join condition

Here is a visualization of taxi drop-off locations, with latitude and longitude binned at a resolution of 7 (1.22km edge length) and colored by aggregated counts within each bin.

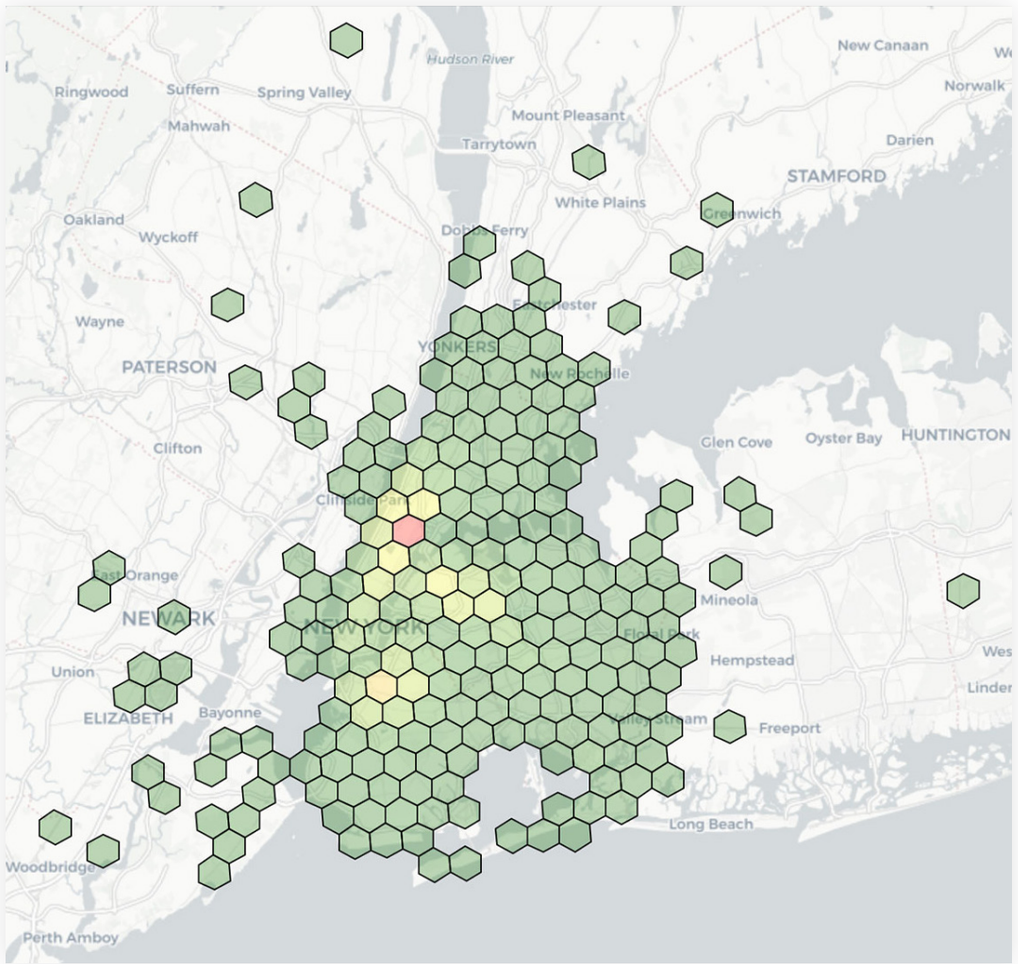


Figure 6: Geospatial visualization of taxi drop-off locations, with latitude and longitude binned at a resolution of 7 (1.22km edge length) and colored by aggregated counts within each bin

Handling spatial formats with Databricks

Geospatial data involves reference points, such as latitude and longitude, to physical locations or extents on the Earth along with features described by attributes. While there are many file formats to choose from, we have picked out a handful of representative vector and raster formats to demonstrate reading with Databricks.

Vector data

Vector data is a representation of the world stored in x (longitude), y (latitude) coordinates in degrees, and also z (altitude in meters) if elevation is considered. The three basic symbol types for vector data are points, lines and polygons. Well-known-text (WKT), GeoJSON and shapefile are some popular formats for storing vector data we highlight below.

Let's read NYC Taxi Zone data with geometries stored as WKT. The data structure we want to get back is a DataFrame that will allow us to standardize with other APIs and available data sources, such as those used elsewhere in the blog. We are able to easily convert the WKT content found in field the_geom into its corresponding JTS Geometry class through the st_geomFromWKT(...) UDF call.

```
%scala
val wktDFText = sqlContext.read.format("csv")
 .option("header", "true")
 .option("inferSchema", "true")
 .load("/ml/blogs/geospatial/nyc_taxi_zones.wkt.csv")

val wktDF = wktDFText.withColumn("the_geom", st_geomFromWKT(col("the_
geom"))).cache
```

GeoJSON is used by many open source GIS packages for encoding a variety of geographic data structures, including their features, properties and spatial extents. For this example, we will read NYC Borough Boundaries with the approach taken depending on the workflow. Since the data is conforming to JSON, we could use the Databricks built-in JSON reader with .option("multiline","true") to load the data with the nested schema.

```
%python
json_df = spark.read.option("multiline","true").json("nyc_boroughs.geojson")
```

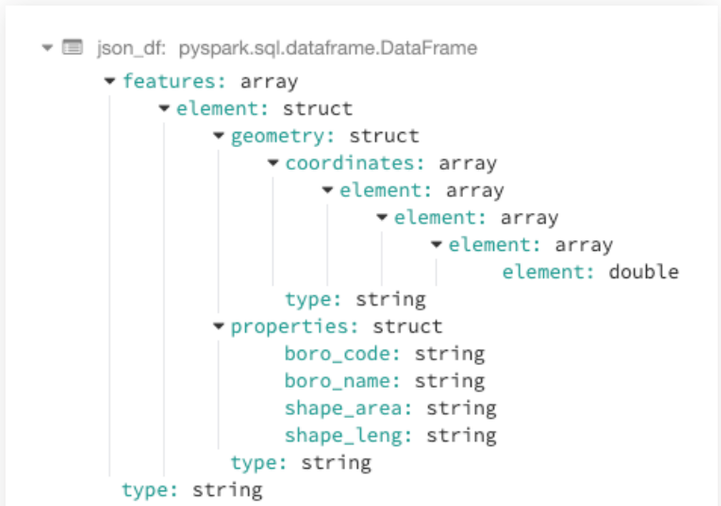


Figure 7: Using the Databricks built-in JSON reader .option("multiline","true") to load the data with the nested schema

From there, we could choose to hoist any of the fields up to top level columns using Spark's built-in explode function. For example, we might want to bring up geometry, properties and type and then convert geometry to its corresponding JTS class, as was shown with the WKT example.

```
%python
from pyspark.sql import functions as F
json_explode_df = ( json_df.select(
 "features",
 "type",
 F.explode(F.col("features.properties")).alias("properties")
).select("*",F.explode(F.col("features.geometry")).alias("geometry")).
drop("features"))

display(json_explode_df)
```

type	properties	geometry
FeatureCollection	object boro_code: 2 boro_name: Bronx shape_area: 1186612476.97 shape_leng: 462958.186921	object coordinates: [[[[-73.89680883223774,40.79580844515979],[-73.89693872998792,40.79563587285357], [-73.89723603843939,40.79572003753707],[-73.89796839783742,40.795644839161994], [-73.89857332665558,40.7960691402596],[-73.89895261832527,40.796227852579634], [-73.89919434249981,40.79650245601821],[-73.89852052071471,40.796936194189776], [-73.89788253240185,40.79711653214705],[-73.89713149795642,40.79679807772831], [-73.89678526341234,40.79632916648710 5],[-73.89680883223774,40.79580844515979]]], [[[-73.88885148496334,40.798706328958765],[-73.8886021869873,40.798650985918705], [-73.8885856250733,40.798706072297094],[-73.88821348851279,40.798665304638554], [-73.88821415282712,40.79866379621751],[-73.88825230744402,40.798577180398 3], [-73.88837251379924,40.79858745625632],[-73.88839250519693,40.79856629726993],

Figure 8: Using the Spark's built-in explode function to raise a field to the top level, displayed within a DataFrame table

We can also visualize the NYC Taxi Zone data within a notebook using an existing DataFrame or directly rendering the data with a library such as Folium, a Python library for rendering spatial data. Databricks File System (DBFS) runs over a distributed storage layer, which allows code to work with data formats using familiar file system standards. DBFS has a FUSE Mount to allow local API calls that perform file read and write operations, which makes it very easy to load data with non-distributed APIs for interactive rendering. In the Python open(...) command below, the "/dbfs/..." prefix enables the use of FUSE Mount.

```
%python
import folium
import json

with open ("/dbfs/ml/blogs/geospatial/nyc_boroughs.geojson", "r") as
myfile:
 boro_data=myfile.read() # read GeoJSON from DBFS using FuseMount

m = folium.Map(
 location=[40.7128, -74.0060],
 tiles='Stamen Terrain',
 zoom_start=12
)
folium.GeoJson(json.loads(boro_data)).add_to(m)
m # to display, also could use displayHTML(...) variants
```

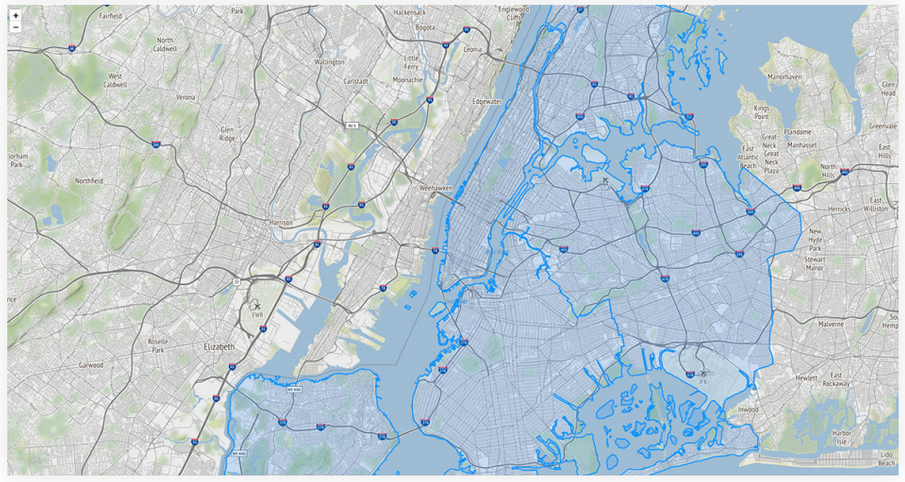


Figure 9: We can also visualize the NYC Taxi Zone data, for example, within a notebook using an existing DataFrame or directly rendering the data with a library such as Folium, a Python library for rendering geospatial data

Shapefile is a popular vector format developed by ESRI that stores the geometric location and attribute information of geographic features. The format consists of a collection of files with a common filename prefix (*.shp, *.shx and *.dbf are mandatory) stored in the same directory. An alternative to shapefile is KML, also used by our customers but not shown for brevity. For this example, let's use NYC Building shapefiles. While there are many ways to demonstrate reading shapefiles, we will give an example using GeoSpark. The built-in ShapefileReader is used to generate the rawSpatialDf DataFrame.

```
%scala
var spatialRDD = new SpatialRDD[Geometry]
spatialRDD = ShapefileReader.readToGeometryRDD(sc, "/ml/blogs/
geospatial/shapefiles/nyc")

var rawSpatialDf = Adapter.toDf(spatialRDD,spark)
rawSpatialDf.createOrReplaceTempView("rawSpatialDf") //DataFrame now
available to SQL, Python, and R
```

By registering rawSpatialDf as a temp view, we can easily drop into pure Spark SQL syntax to work with the DataFrame, to include applying a UDF to convert the shapefile WKT into Geometry.

```
%sql
SELECT *,
 ST_GeomFromWKT(geometry) AS geometry -- GeoSpark UDF to convert WKT to
Geometry
FROM rawspatialdf
```

Additionally, we can use Databricks' built-in visualization for in-line analytics, such as charting the tallest buildings in NYC.

```
%sql
SELECT name,
 round(Cast(num_floors AS DOUBLE), 0) AS num_floors --String to Number
FROM rawspatialdf
WHERE name  ''
ORDER BY num_floors DESC LIMIT 5
```

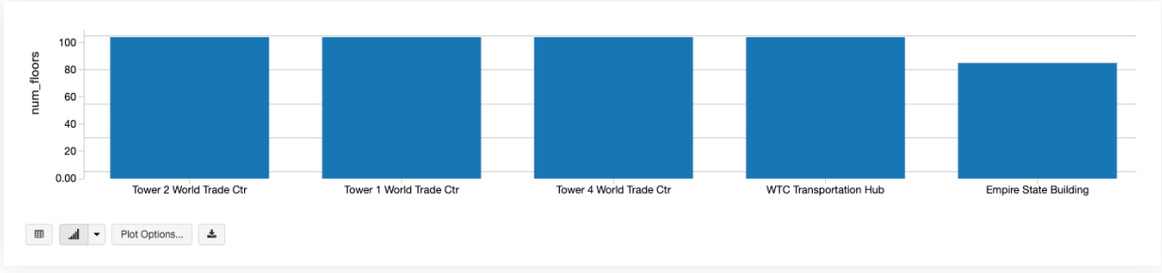


Figure 10: A Databricks built-in visualization for in-line analytics charting, for example, the tallest buildings in NYC

Raster data

Raster data stores information of features in a matrix of cells (or pixels) organized into rows and columns (either discrete or continuous). Satellite images, photogrammetry and scanned maps are all types of raster-based Earth Observation (EO) data.

The following Python example uses RasterFrames, a DataFrame-centric spatial analytics framework, to read two bands of GeoTIFF Landsat-8 imagery (red and near-infrared) and combine them into Normalized Difference Vegetation Index. We can use this data to assess plant health around NYC. The rf_ipython module is used to manipulate RasterFrame contents into a variety of visually useful forms, such as below where the red, NIR and NDVI tile columns are rendered with color ramps, using the Databricks built-in displayHTML(...) command to show the results within the notebook.

```
%python
# construct a CSV "catalog" for RasterFrames `raster` reader
# catalogs can also be Spark or
```

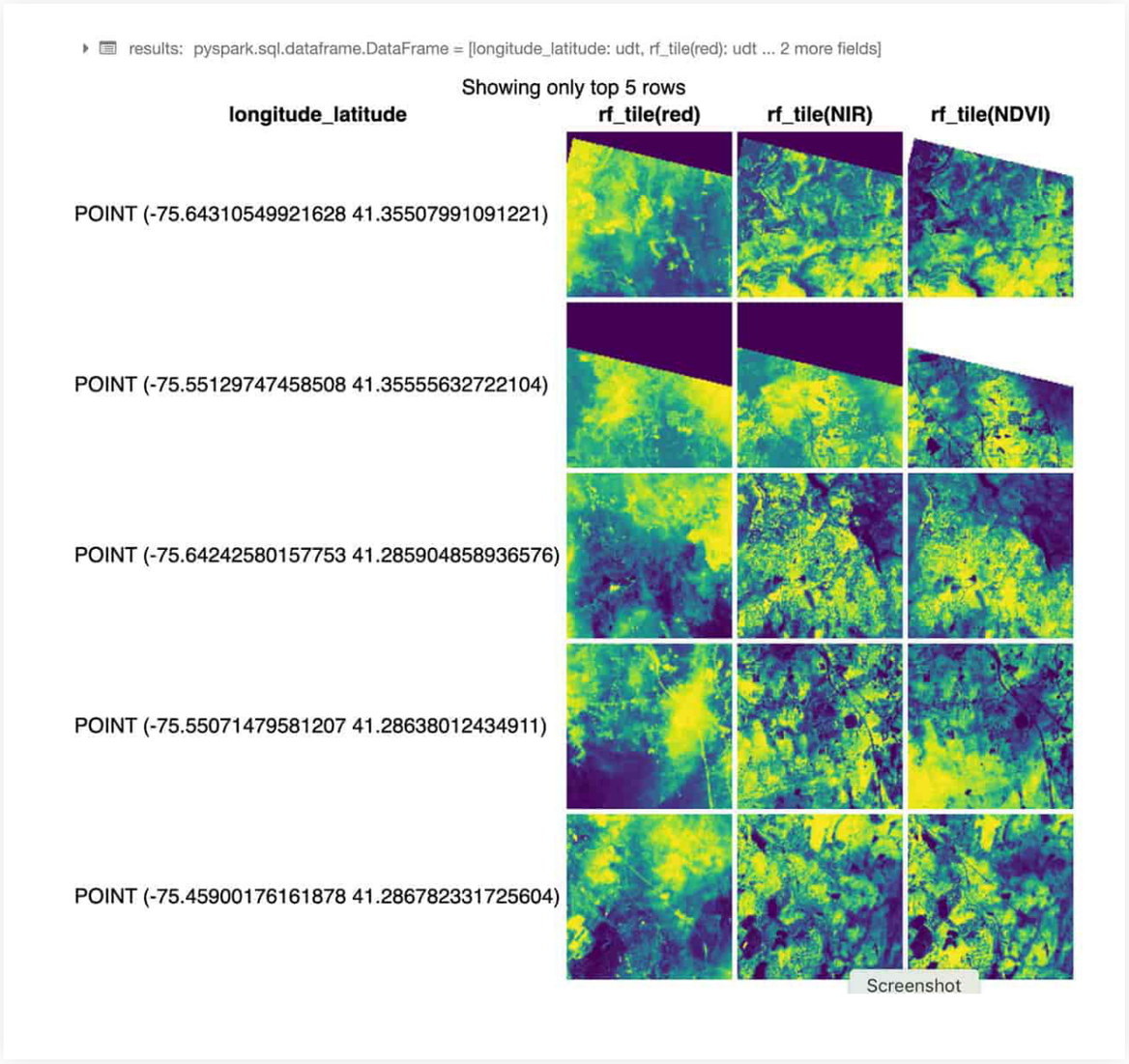


Figure 11: RasterFrame contents can be filtered, transformed, summarized, resampled and rasterized through over 200 raster and vector functions

Through its custom Spark DataSource, RasterFrames can read various raster formats, including GeoTIFF, JP2000, MRF and HDF, from an array of services. It also supports reading the vector formats GeoJSON and WKT/WKB. RasterFrame contents can be filtered, transformed, summarized, resampled and rasterized through over 200 raster and vector functions, such as st_reproject(...) and st_centroid(...) used in the example above. It provides APIs for Python, SQL and Scala as well as interoperability with Spark ML.

Geodatabases

Geodatabases can be file based for smaller scale data or accessible via JDBC/ODBC connections for medium scale data. You can use Databricks to query many SQL databases with the built-in JDBC/ODBC Data Source. Connecting to PostgreSQL is shown below and is commonly used for smaller scale workloads by applying PostGIS extensions. This pattern of connectivity allows customers to maintain as-is access to existing databases.

```
%scala
display(
  sqlContext.read.format("jdbc")
    .option("url", jdbcUrl)
    .option("driver", "org.postgresql.Driver")
    .option("dbtable",
    """(SELECT * FROM yellow_tripdata_staging
    OFFSET 5 LIMIT 10) AS t""") //predicate pushdown
   .option("user", jdbcUsername)
   .option("jdbcPassword", jdbcPassword)
  .load)
```

vendor_id	tpep_pickup_datetime	tpep_dropoff_datetime	passenger_count	trip_distance	rate_code_id	store_and_fwd_flag	pickup_location_id	dropoff_location_id	payment_type	fare_amount
2	2019-01-06 16:27:40	2019-01-06 16:29:47	5	.16	1	N	142	142	4	-3
2	2019-01-06 16:27:40	2019-01-06 16:29:47	5	.16	1	N	142	142	2	3
2	2019-01-06 16:51:27	2019-01-06 17:05:55	5	1.99	1	N	239	230	2	11
1	2019-01-06 16:38:49	2019-01-06 16:58:05	1	2.10	1	N	164	163	2	13
1	2019-01-06 16:59:54	2019-01-06 17:09:33	4	1.40	1	N	163	186	2	8
2	2019-01-06 16:25:58	2019-01-06 16:35:36	3	1.77	1	N	137	90	1	8.5
2	2019-01-06 16:42:45	2019-01-06 16:47:05	3	.67	1	N	68	234	2	5
2	2019-01-06 16:50:21	2019-01-06 16:57:03	2	1.09	1	N	234	100	1	6.5

Getting started with geospatial analysis on Databricks

Businesses and government agencies seek to use spatially referenced data in conjunction with enterprise data sources to draw actionable insights and deliver on a broad range of innovative use cases. In this blog we demonstrated how the Databricks Unified Data Analytics Platform can easily scale geospatial workloads, enabling our customers to harness the power of the cloud to capture, store and analyze data of massive size.

In an upcoming blog, we will take a deep dive into more advanced topics for geospatial processing at-scale with Databricks. You will find additional details about the spatial formats and highlighted frameworks by reviewing Data Prep Notebook, GeoMesa + H3 Notebook, GeoSpark Notebook, GeoPandas Notebook, and RasterFrames Notebook. Also, stay tuned for a new section in our documentation specifically for geospatial topics of interest.

About Databricks

Databricks is the lakehouse company. More than 7,000 organizations worldwide — including Comcast, Condé Nast, H&M and over 50% of the Fortune 500 — rely on the Databricks Lakehouse Platform to unify their data, analytics and AI. Databricks is headquartered in San Francisco, with offices around the globe. Founded by the original creators of Apache Spark™, Delta Lake and MLflow, Databricks is on a mission to help data teams solve the world's toughest problems. To learn more, follow Databricks on Twitter, LinkedIn and Facebook.

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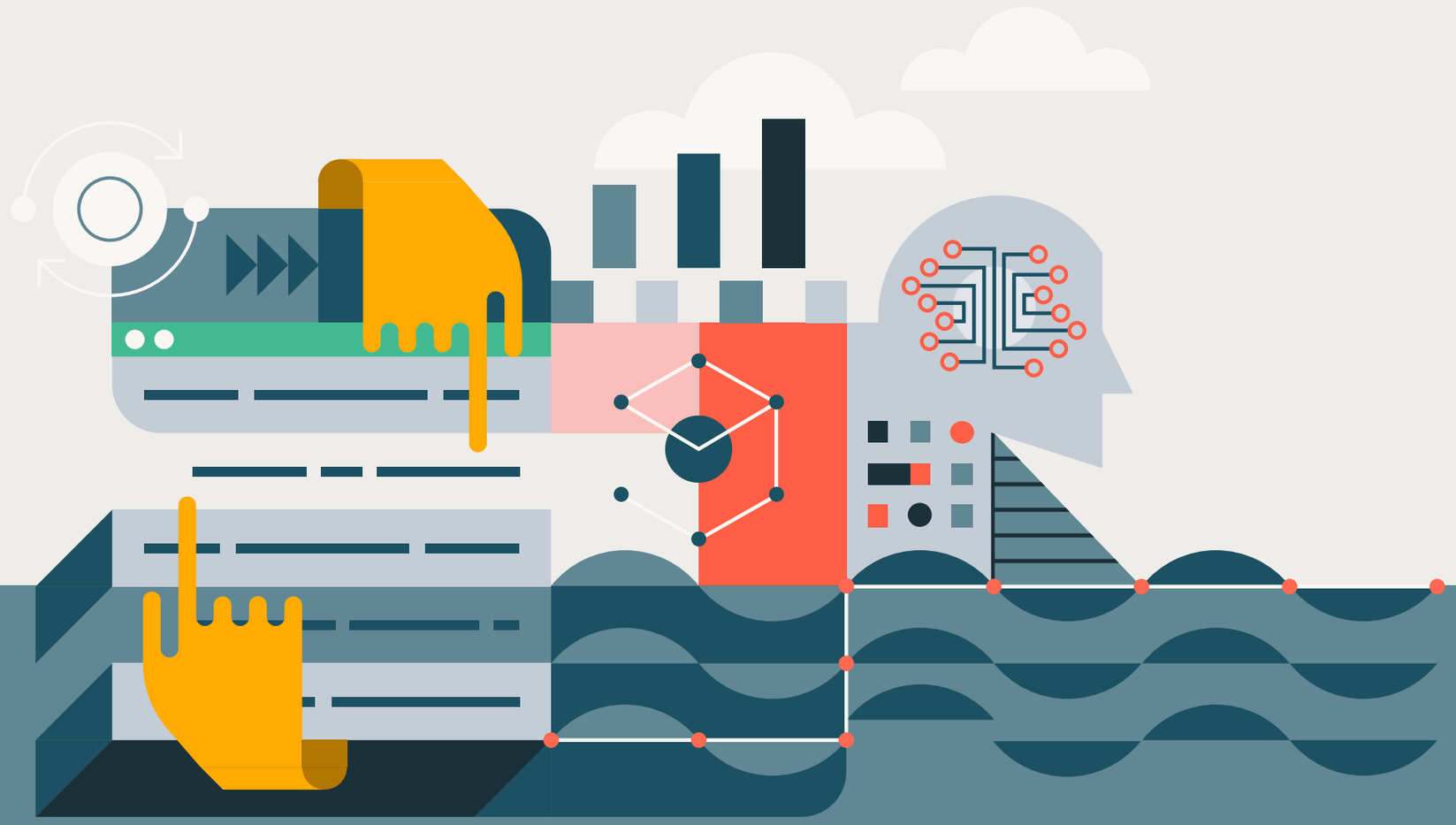

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