Python for High Performance Data Analytics

Prerequisites

- Basic proficiency in Python (variables, flow control, functions)
- Basic grasp of descriptive statistics (such as minimum, maximum, median, arithmetic mean…)
- Basic knowledge of NumPy
- Basic knowledge of some plotting package (Matplotlib, Seaborn, Holoviz…)

20 min | filename

Tabular data (aka Dataframes)

Questions

- What are series and dataframes?
- What do we mean by tidy and untidy data?
- What packages are available in Python to handle dataframes?

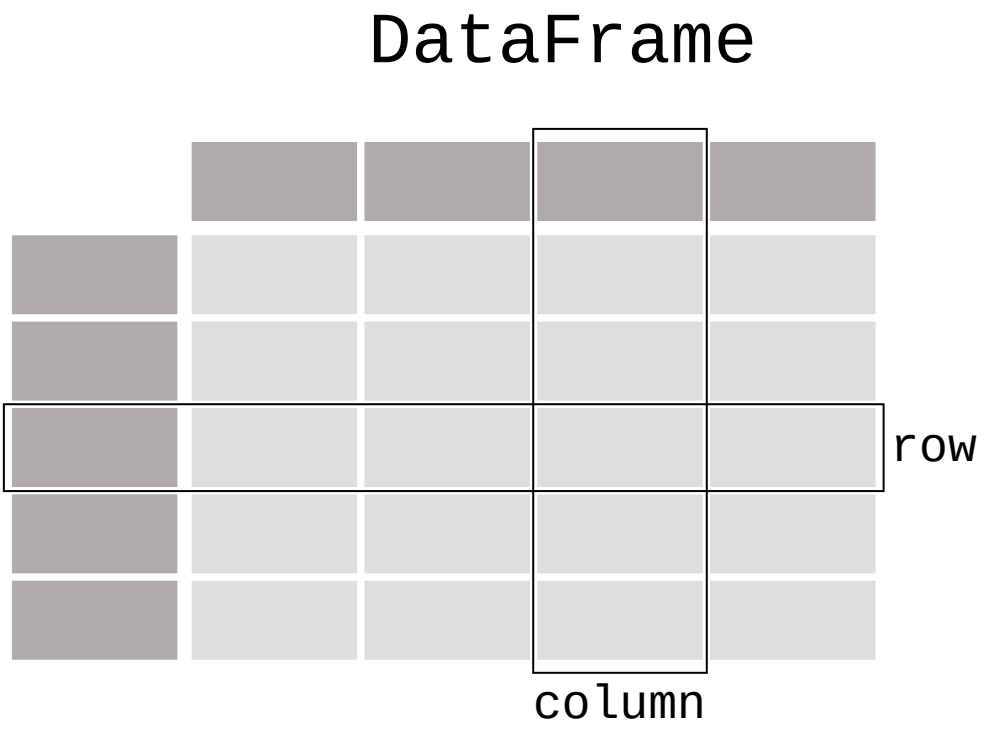
Objectives

- Learn how to manipulate dataframes in Pandas
- Lazy and eager dataframes in Polars

This episode will give an introduction to the concepts of *Series* and *DataFrame* and how they can be manipulated using different Python packages.

Series and dataframes

A collection of observations (e.g. a time series or simply a set of observations of a feature of a phenomenon) can be represented by a homogeneous vector, i.e. an array where all the elements are of the same type. This is known as a *Series* in many frameworks. Several series (of different types) can be used as columns of a tabular structure called a *Dataframe*, as depicted in the figure below



Tidy vs untidy dataframes

Let us look at the following two dataframes:

Untidy format | Tidy format

	Runner	400	800	1200	1500
0	Runner 1	64	128	192	240
1	Runner 2	80	160	240	300
2	Runner 3	96	192	288	360

Most tabular data is either in a tidy format or a untidy format (some people refer them as the long format or the wide format). The main differences are summarised below:

- In untidy (wide) format, each row represents an observation consisting of multiple variables and each variable has its own column. This is intuitive and easy for us to understand and make comparisons across different variables, calculate statistics, etc.
- In tidy (long) format , i.e. column-oriented format, each row represents only one variable of the observation, and can be considered “computer readable”. When it comes to data analysis using Pandas, the tidy format is recommended:
- Each column can be stored as a vector and this not only saves memory but also allows for vectorized calculations which are much faster.
- It’s easier to filter, group, join and aggregate the data.

Imagine, for example, that you would like to compute the speed as `speed=distance/time`. The untidy format would make this much clunkier, as:

- The distances are encoded as column names, not as data points (rows)
- The speed would have to be stored in a new dataframe since it would not fit in that data structure.

In comparison, in a tidy dataframe, this computation would be a simple operation between two columns.

> **Tip**
>
> Recovering a wide dataframe from a tidy one is commonly referred to as *pivoting*. Most dataframe libraries provide a `pivot()` or `pivot_table` function.

Pandas & Polars

Historically, Pandas has been the go-to package to handle dataframes in Python. It is based on NumPy (each column is a Numpy vector) and has been the traditional workhorse for tabular data, with a stable API and a large ecosystem built around it, including the Seaborn statistical plotting framework. More recently, Polars was introduced as a more modern and faster alternative to handle dataframes. It is written in Rust and supports out of the box out of core evaluation (i.e. does not need loading the whole dataset in memory), lazy evaluation of queries and automatically uses multiple threads. Moreover, experimental GPU support is available through cuDF. In the remainder of this episode, the NYC taxi will be used to showcase how datasets can be accessed, summarised and manipulated in both Pandas and Polars. The dataset can be

uet format from the link above (the file for the month of January was used in taset contains information about taxi trips performed in New York, such as the ID of the vendor, the total fare, pickup and drop-off time and location (expressed as an ID), type of payment, whether additional fees were charged and more.

Opening a dataset

Assuming the file is called `yellow_tripdata_2025-01.parquet`, the dataset can be opened as:

Pandas | Polars

```
import pandas as pd
df = pd.read_parquet("yellow_tripdata_2025-01.parquet")
```

Description and summarisation

We can get a first understanding of the contents of a dataframe by printing the first few lines, the "schema" (i.e. the number and type of each column) and summary statistics as follows:

Pandas | Polars

```
df.head()
```

Output

```
   VendorID tpep_pickup_datetime tpep_dropoff_datetime  ...  congestion_surcharge  Airport_fee  cbd
0         1  2025-01-01 00:18:38   2025-01-01 00:26:59  ...                   2.5          0.0
1         1  2025-01-01 00:32:40   2025-01-01 00:35:13  ...                   2.5          0.0
2         1  2025-01-01 00:44:04   2025-01-01 00:46:01  ...                   2.5          0.0
3         2  2025-01-01 00:14:27   2025-01-01 00:20:01  ...                   0.0          0.0
4         2  2025-01-01 00:21:34   2025-01-01 00:25:06  ...                   0.0          0.0
```

```
df.info()
```

Output

```
RangeIndex: 3475226 entries, 0 to 3475225
Data columns (total 20 columns):
 #   Column                 Dtype
---  ------                 -----
 0   VendorID               int32
 1   tpep_pickup_datetime   datetime64[us]
 2   tpep_dropoff_datetime  datetime64[us]
 3   passenger_count        float64
 4   trip_distance          float64
 5   RatecodeID             float64
 6   store_and_fwd_flag     object
 7   PULocationID           int32
 8   DOLocationID           int32
 9   payment_type           int64
 10  fare_amount            float64
 11  extra                  float64
 12  mta_tax                float64
 13  tip_amount             float64
 14  tolls_amount           float64
 15  improvement_surcharge  float64
 16  total_amount           float64
 17  congestion_surcharge   float64
 18  Airport_fee            float64
 19  cbd_congestion_fee     float64
dtypes: datetime64[us](2), float64(13), int32(3), int64(1), object(1)
memory usage: 490.5+ MB
```

```
df.describe()
```

Output

```
           VendorID        tpep_pickup_datetime       tpep_dropoff_datetime  ...  congestion_surcha
count  3.475226e+06                     3475226                     3475226  ...          2.935077e
mean   1.785428e+00  2025-01-17 11:02:55.910964  2025-01-17 11:17:56.997901  ...          2.225237e
min    1.000000e+00         2024-12-31 20:47:55         2024-12-18 07:52:40  ...         -2.500000e
25%    2.000000e+00         2025-01-10 07:59:01  2025-01-10 08:15:29.500000  ...          2.500000e
50%    2.000000e+00         2025-01-17 15:41:33         2025-01-17 15:59:34  ...          2.500000e
75%    2.000000e+00         2025-01-24 19:34:06         2025-01-24 19:48:31  ...          2.500000e
max    7.000000e+00         2025-02-01 00:00:44         2025-02-01 23:44:11  ...          2.500000e
std    4.263282e-01                         NaN                         NaN  ...          9.039932e

[8 rows x 19 columns]
```

Indexing

We can index data in the dataframe as follows:

Skip to content

Pandas | Polars

```
# With this we can select a column
df['VendorID'] # Could also be df.VendorID
```

Output

```
0          1
1          1
2          1
3          2
4          2
          ..
3475221    2
3475222    2
3475223    2
3475224    2
3475225    2
```

```
# Get a row
df.iloc[1000,:]
```

Output

```
VendorID                                2
tpep_pickup_datetime     2025-01-01 00:08:06
tpep_dropoff_datetime    2025-01-01 00:16:20
passenger_count                        4.0
trip_distance                         1.53
RatecodeID                             1.0
store_and_fwd_flag                       N
PULocationID                           114
DOLocationID                            90
payment_type                             1
fare_amount                           10.0
extra                                  1.0
mta_tax                                0.5
tip_amount                            2.25
tolls_amount                           0.0
improvement_surcharge                  1.0
total_amount                         17.25
congestion_surcharge                   2.5
Airport_fee                            0.0
cbd_congestion_fee                     0.0
Name: 1000, dtype: object
>>> df.iloc[1000,:]
VendorID                                2
tpep_pickup_datetime     2025-01-01 00:08:06
tpep_dropoff_datetime    2025-01-01 00:16:20
passenger_count                        4.0
trip_distance                         1.53
RatecodeID                             1.0
store_and_fwd_flag                       N
PULocationID                           114
DOLocationID                            90
payment_type                             1
fare_amount                           10.0
extra                                  1.0
mta_tax                                0.5
tip_amount                            2.25
tolls_amount                           0.0
improvement_surcharge                  1.0
total_amount                         17.25
congestion_surcharge                   2.5
Airport_fee                            0.0
cbd_congestion_fee                     0.0
```

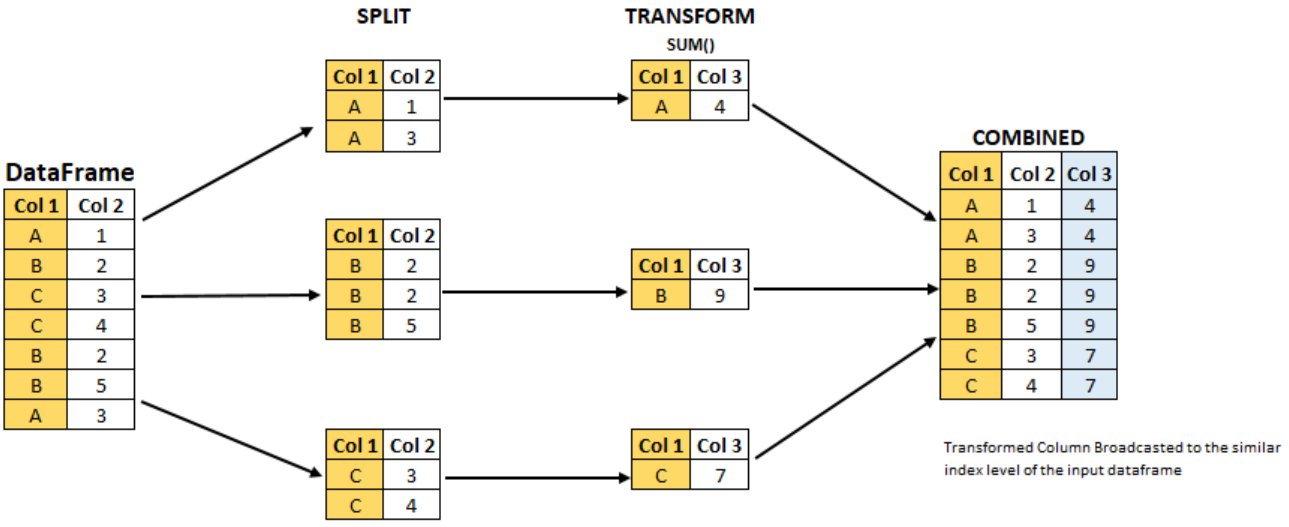
In both cases, a similar syntax can be used to do in-place modification (e.g. `df[row][column]=...`). Please note that this kind of replacement carries a big performance penalty, which is designed to do column-wide operations with minimal overhead. This is commonly achieved through the expression API, as detailed in the next section.

Common workflows

It is quite common to stratify (i.e. divide the samples into a number of groups based on categorical variables) to produce descriptive statistics (i.e. statistics that provide a summary of the samples and do not aim to predict anything regarding the population it comes from). This is commonly achieved through a `group-by` workflow, where the following happens:

- Splitting: data is partitioned into different groups based on some criterion
- Applying: applying a function/performing a calculation to each group
- Combining: assembling a dataframe (of potentially any size) with the results.

This is type of workflow is represented below.



SOURCE: EARTH AND ENVIRONMENTAL DATA SCIENCE

As an example, let us try to to compute the total fare for each hour, split by payment type.

Pandas | Polars

```
#First let us extract the hour from the tpep_pickup_datetime column
df["hour"] = df['tpep_pickup_datetime'].dt.hour

hourly_fare = (
  df.groupby(['hour', 'payment_type'], observed=False)['fare_amount']
  .sum()
  .reset_index()
  .sort_values(['hour', 'payment_type'])
```

Output

```
     hour  payment_type  fare_amount
0       0             0    352227.86
1       0             1   1088201.12
2       0             2    156546.07
3       0             3      3537.91
4       0             4      3941.24
..    ...           ...          ...
116    23             0    534063.76
117    23             1   1618143.37
118    23             2    219991.22
119    23             3      4765.54
120    23             4      3293.61
```

The `groupby` statement is used to stratify the `fare_amount` column by hour and payment type. Then the amounts per hour and type get summed and sorted according to time and payment type.

Idiomatic Polars

Polars introduces a few variations to dataset operations compared to the traditional Pandas approach. In particular, a domain-specific language (DSL) was developed, where *expressions* are written to represent dataset operations and *context*s provide the environment where they produce a result.

Expressions

Let's say that we created a `trip_duration_sec` column in our NYC cab database and, given the `trip_distance` column, we want to compute the average speed. In Polars, this can be achieved with:

```
pl.col('trip_distance') / pl.col(`trip_duration_sec`)
```

This is a lazy representation of an operation we want to perform, which can be further manipulated or just printed. For it to actually produce data, a *context* is needed.

Contexts

The same Polars expression can produce different results depending on the context where it is used. Four common contexts include:

- `select`

- `filter`
- `group_by`

Both `select` and `with_columns` can produce new columns, which may be aggregations, combinations of other columns, or literals. The difference between the two is that `select` only includes the columns contained in its input expression, whereas `with_columns` returns a new dataframe which contains all the columns from the original dataframe and the new ones created by the expression. To exemplify, using our earlier example of computing the average speed during a trip, using `select` would yield a single column, whereas `with_columns` would return the original dataframe with an additional column called `trip distance`:

```
df.select(pl.col('trip_distance')/pl.col('trip_duration_sec')*3600)
shape: (3_475_226, 1)
┌─────────────────┐
│ trip_distance   │
│ ---             │
│ f64             │
╞═════════════════╡
│ 11.497006       │
│ 11.764706       │
│ 18.461538       │
│ 5.60479         │
│ 11.207547       │
│ …               │
│ 13.68899        │
│ 19.42398        │
│ 9.879418        │
│ 9.339901        │
│ 12.781395       │
└─────────────────┘
```

```
df.with_columns((pl.col('trip_distance')/pl.col('trip_duration_sec')*3600).alias("avg_s
eed_mph"))
shape: (3_475_226, 22)
```

VendorID	tpep_pickup_datetime	tpep_dropoff_datetime	passenger_count	…	Airport_fee	cbd_congestion_fee	trip_duration_sec	avg_mp
i32	---	---	i64		f64	---	---	---
	datetime [µs]	datetime [µs]				f64	i64	f64
1	2025-01-01 00:18:38	2025-01-01 00:26:59	1	…	0.0	0.0	501	11.4
1	2025-01-01 00:32:40	2025-01-01 00:35:13	1	…	0.0	0.0	153	11.7
1	2025-01-01 00:44:04	2025-01-01 00:46:01	1	…	0.0	0.0	117	18.4
2	2025-01-01 00:14:27	2025-01-01 00:20:01	3	…	0.0	0.0	334	5.6
2	2025-01-01 00:21:34	2025-01-01 00:25:06	3	…	0.0	0.0	212	11.1
…	…	…	…	…	…	…	…	…
2	2025-01-31 23:01:48	2025-01-31 23:16:29	null	…	null	0.75	881	13.4
2	2025-01-31 23:50:29	2025-02-01 00:17:27	null	…	null	0.75	1618	19.4
2	2025-01-31 23:26:59	2025-01-31 23:43:01	null	…	null	0.75	962	9.8
2	2025-01-31 23:14:34	2025-01-31 23:34:52	null	…	null	0.75	1218	9.3
2	2025-01-31 23:56:42	2025-02-01 00:07:27	null	…	null	0.0	645	12.7

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ext filters the rows of a dataframe based on one (or more) expressions which lean, e.g.

```
df.filter(pl.col('avg_speed_mph') < 1)
shape: (104_410, 22)
```

VendorID	tpep_pickup_datetime	tpep_dropoff_datetime	passenger_count	…	Airport_fee	cbd_congestion_fee	trip_duration_sec	avg_m
i32	datetime[μs]	datetime[μs]	i64		f64	f64	i64	f64
2	2025-01-01 00:37:43	2025-01-01 00:37:53	1	…	0.0	0.0	10	0.0
2	2025-01-01 00:57:08	2025-01-01 00:57:16	3	…	0.0	0.0	8	0.0
1	2025-01-01 00:27:40	2025-01-01 00:59:30	1	…	0.0	0.0	1910	0.0
2	2025-01-01 00:56:49	2025-01-01 00:56:54	4	…	0.0	0.0	5	0.0
1	2025-01-01 00:42:42	2025-01-01 00:42:44	0	…	0.0	0.0	2	0.0
…	…	…	…	…	…	…	…	…
1	2025-01-31 23:59:17	2025-02-01 00:03:43	null	…	null	0.75	266	0.0
1	2025-01-31 23:17:38	2025-01-31 23:35:58	null	…	null	0.75	1100	0.0
2	2025-01-31 23:39:25	2025-01-31 23:42:06	null	…	null	0.0	161	0.0
1	2025-01-31 23:30:42	2025-01-31 23:31:06	null	…	null	0.75	24	0.0
1	2025-01-31 23:10:25	2025-01-31 23:36:21	null	…	null	0.75	1556	0.0

The `group_by` context behaves like its Pandas counterpart.

Transformations

A `join` operation combines columns from one or more dataframes into a new dataframe. There are different joining strategies, which influence how columns are combined and what rows are included in the final set. A common type is the *equi* join, where rows are matched by a key expression. Let us clarify this with an example. The `df` dataframe does not include specific coordinates for each pickup and drop-off, rather only a `PULocationID` and a `DOLocationID`. There is a `taxy_zones_xy.csv` file that contains, for each `LocationID`, the latitude (X) and longitude (Y) of each location, as well as the name of zone and borough:

```
lookup_df = pl.read_csv('taxy_zones_xy.csv', has_header=True)
lookup_df.head()
```

```
┌────────────┬───────────┬──────────┬──────────────────────┬─────────────┐
│ LocationID ┆ X         ┆ Y        ┆ zone                 ┆ borough     │
│ ---        ┆ ---       ┆ ---      ┆ ---                  ┆ ---         │
│ i64        ┆ f64       ┆ f64      ┆ str                  ┆ str         │
╞════════════╪═══════════╪══════════╪══════════════════════╪═════════════╡
│ 1          ┆ -74.176786 ┆ 40.689516 ┆ Newark Airport       ┆ EWR         │
│ 2          ┆ -73.826126 ┆ 40.625724 ┆ Jamaica Bay          ┆ Queens      │
│ 3          ┆ -73.849479 ┆ 40.865888 ┆ Allerton/Pelham Gardens ┆ Bronx    │
│ 4          ┆ -73.977023 ┆ 40.724152 ┆ Alphabet City        ┆ Manhattan   │
│ 5          ┆ -74.18993  ┆ 40.55034  ┆ Arden Heights        ┆ Staten Island │
└────────────┴───────────┴──────────┴──────────────────────┴─────────────┘
```

This can be used to append these columns to the original df to have some form of geographical data as follows (e.g. for the `PULocationID`):

```
df = df.join(lookup_df, left_on='PULocationID', right_on='LocationID', how='left'
, suffix='_pickup')
```

In the line above, `left_on` is used to indicate the *key* in the original dataframe, `right_on` is used to specify the *key* in the `lookup_df` dataframe, `how=left` means that the columns from the second dataframe will be added to the first (and not the other way around) and `suffix` is what will be added to the names of the joined columns (i.e., df will contain columns called `X_pickup`, `Y_pickup`, `zone_pickup` and `borough_pickup`). More information on join operations can be found here.

Exercises

Joining geographical data

We have already seen how to add actual latitude and longitude for the pickups. Now do the same for the drop-offs!

Solution

```
df = df.join(lookup_df, left_on='DOLocationID', right_on='LocationID', how='left'
, suffix='_dropoff')
```

Feature engineering: enriching the dataset

We want to understand a bit more of the traffic in the city by creating new features (i.e. columns), in particular:

- Split the pickup datetime into hour, minute, day of the week and month to indentify daily, weekly and monthly trends
- Compute the average speed as an indicator of congestion (low speed -> traffic jam)
- Stratify the trip distance and fare by zone to identify how expensive different zones are. Below is a skeleton of the code, where some lines have been blanked out for you to fill (marked with `TODO:...`)

```
import polars as pl
raw_df = pl.read_parquet('yellow_tripdata_2025-01.parquet')
df = raw_df.with_columns([
    pl.col("tpep_pickup_datetime").dt.hour().alias("pickup_hour"),
    #TODO: do this for the minute
    pl.col("tpep_pickup_datetime").dt.day_of_week().alias("pickup_dow"),   # Mon=0 … Sun=6
    pl.col("tpep_pickup_datetime").dt.month().alias("pickup_month"),
    # Trip duration in seconds
    (pl.col("tpep_dropoff_datetime") - pl.col("tpep_pickup_datetime"))
        .dt.total_seconds()
        .alias("trip_duration_sec"),
])

df = df.with_column(
    #TODO: add expression for average velocity here
    .replace_nan(None)                        # protect against div-by-zero
    .alias("avg_speed_mph")
)

# Compute per-pickup-zone statistics once
zone_stats = (
    df.groupby("PULocationID")
      .agg([
          pl.mean("fare_amount").alias("zone_avg_fare"),
          #TODO: do the same for the trip distance here
          pl.count().alias("zone_trip_cnt"),
      ])
      .rename({"PULocationID": "pickup_zone_id"})   # avoid name clash later
)

# Join those stats back onto the original rows
df = df.join(zone_stats, left_on="PULocationID", right_on="pickup_zone_id", how="left")
```

While we haven't covered the `join` instruction earlier, its main role is to "spread" the `zone_stats` over all the rides in the original dataframe (i.e. write the `zone_avg_fare` on each ride in `df`). `join` has its roots in relational databases, where different tables can be merged based on a common column.

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Solution

```
import polars as pl
raw_df = pl.read_parquet('yellow_tripdata_2025-01.parquet')
df = raw_df.with_columns([
    pl.col("tpep_pickup_datetime").dt.hour().alias("pickup_hour"),
    pl.col("tpep_pickup_datetime").dt.minute().alias("pickup_minute"),
    pl.col("tpep_pickup_datetime").dt.day_of_week().alias("pickup_dow"),    # Mon=0 … Sun=6
    pl.col("tpep_pickup_datetime").dt.month().alias("pickup_month"),
    # Trip duration in seconds
    (pl.col("tpep_dropoff_datetime") - pl.col("tpep_pickup_datetime"))
        .dt.seconds()
        .alias("trip_duration_sec"),
])

df = df.with_column(
    (
        pl.col("trip_distance") /
        (pl.col("trip_duration_sec") / 3600)   # seconds → hours
    )
    .replace_nan(None)                         # protect against div-by-zero
    .alias("avg_speed_mph")
)

# Compute per-pickup-zone statistics once
zone_stats = (
    df.groupby("PULocationID")
      .agg([
          pl.mean("fare_amount").alias("zone_avg_fare"),
          pl.mean("trip_distance").alias("zone_avg_dist"),
          pl.count().alias("zone_trip_cnt"),
      ])
      .rename({"PULocationID": "pickup_zone_id"})   # avoid name clash later
)

# Join those stats back onto the original rows
df = df.join(zone_stats, left_on="PULocationID", right_on="pickup_zone_id", how="left")
```

More feature engineering!

Similarly to the exercise above, define the following features in the data:

- `pickup_hour` extracted from `tpep_pickup_time`
- `is_weekend`, a Boolean value for each trip
- `avg_speed_mph`, exactly as before
- `tip_to_fare_ratio`, dividing the tip amount by the total fare. Be careful with division by 0
- `fare_per_mile`, dividing the total fare by the distance
- `dist_per_passenger`, the average distance travelled by each passenger (sum of all trip distances divided by number of trips)
- `speed_per_pickup_area`, the average velocity stratified by pickup location
- `dropoff_trip_count`, count of trips stratified per dropoff location

Skip to content

Solution

```
import polars as pl
raw_df = pl.read_parquet("yellow_tripdata_2025-01.parquet")
df = raw_df.with_columns([
    # 1. pickup_hour
    pl.col("tpep_pickup_datetime").dt.hour().alias("pickup_hour"),

    # 2. is_weekend (Sat=5, Sun=6)
    pl.col("tpep_pickup_datetime")
      .dt.day_of_week()
      .is_in([5, 6])
      .alias("is_weekend"),

    # 3. trip_duration_sec
    (pl.col("tpep_dropoff_datetime") - pl.col("tpep_pickup_datetime"))
        .dt.seconds()
        .alias("trip_duration_sec"),

    # 4. avg_speed_mph
    (
        pl.col("trip_distance") /
        (pl.col("trip_duration_sec") / 3600)
    )
    .replace_nan(None)                      # protect against div-by-zero
    .alias("avg_speed_mph"),

    # 5. tip_to_fare_ratio
    (pl.col("tip_amount") / pl.col("fare_amount"))
        .replace_inf(None)
        .replace_nan(None)
        .alias("tip_to_fare_ratio"),

    # 6. fare_per_mile
    (pl.col("fare_amount") / pl.col("trip_distance"))
        .replace_inf(None)
        .replace_nan(None)
        .alias("fare_per_mile"),

    # 7. dist_per_passenger
    (pl.col("trip_distance") / pl.col("passenger_count"))
        .replace_inf(None)
        .replace_nan(None)
        .alias("dist_per_passenger"),
])

dropoff_stats = (
    df.groupby("DOLocationID")
      .agg([
          pl.mean("avg_speed_mph").alias("dropoff_avg_speed"),
          pl.count().alias("dropoff_trip_cnt"),
      ])
      .rename({"DOLocationID": "dropoff_zone_id"})   # avoid name clash later
)

-zone stats back onto every row
ropoff_stats, left_on="DOLocationID", right_on="dropoff_zone_id", how="left")
```

Summary

We have seen how to deal with common workflows in both Pandas and Polars, starting from basic tasks like opening a dataset and inspecting it to performing split-apply-combine pipelines. We have seen how to use Polars to manipulate datasets and perform some basic feature engineering.

> Keypoints
>
> - Dataframes are combinations of series
> - Both Pandas and Polars can be used to manipulate them
> - The expression API in Polars allows to perform advanced operations with a simple DSL.

See also

There is a lot more to Polars than what we covered in this short introduction. For example, queries like the ones we introduced can be performed lazily, i.e. just declared and then run all together, giving the backend a chance to optimise them. This can dramatically improve performance in the case of complex queries. For this and a lot more, we refer you to the official documentation.

Storage & serialisation backends

> Questions
>
> - What syntax is used to make a lesson?
> - How do you structure a lesson effectively for teaching?
> - `questions` are at the top of a lesson and provide a starting point for what you might learn. It is usually a bulleted list.

> Objectives
>
> - Show a complete lesson page with all of the most common structures.
> - …
>
> This is also a holdover from the carpentries-style. It could usually be left off.

The introduction should be a high level overview of what is on the page and why it is interesting.

The lines below (only in the source) will set the default highlighting language for the entire page.

Skip to content

A section.

Discussion

Discuss the following.

- A discussion section
- Another discussion topic

Section

```
print("hello world")
# This uses the default highlighting language
```

```
print("hello world)
```

Exercises: description

Exercise Topic-1: imperative description of exercise

Exercise text here.

Solution

Solution text here

Summary

A Summary of what you learned and why it might be useful. Maybe a hint of what comes next.

See also

- Other relevant links
- Other link

Keypoints

- What the learner should take away
- point 2
- …

This is another holdover from the carpentries style. This perhaps is better done in a “summary” section.

Visualisations and dashboards

Questions

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- Show a complete lesson page with all of the most common structures.
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Skip to content

1: imperative description of exercise

Exercise text here.

Solution

Solution text here

Summary

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- Other relevant links
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- point 2
- …

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Benchmarking

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Solution text here

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Multithreading

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Objectives

- Show a complete lesson page with all of the most common structures.
- …

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Exercises: description

Skip to content

1: imperative description of exercise

Exercise text here.

Solution

Solution text here

Summary

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Dask

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Skip to content

eference

Instructor’s guide

Why we teach this lesson

Intended learning outcomes

Timing

Preparing exercises

e.g. what to do the day before to set up common repositories.

Other practical aspects

Interesting questions you might get

Typical pitfalls

What to expect from this course

> Discussion
>
> How large are the datasets you are working with?

Both for classical machine/deep learning and (generative) AI, the amount of data needed to train ever-growing models is becoming bigger and bigger. Moreover, great strides in both hardware and software development for high performance computing (HPC) applications allow for large scale computations that were not possible before. This course focuses on high performance data analytics (HPDA). The data can come from simulations or experiments (or just generally available datasets), and the goal is to pre-process, analyse and visualise it. The lesson introduces some of the modern Python stack for data analytics, dealing with packages such as Pandas, Polars, multithreading and Dask, as well as Streamlit for large-scale data visualisations.

Learning outcomes

This lesson provides a broad overview of methods to work with large datasets using tools and libraries from the Python ecosystem. Since this field is fairly extensive, we will try to expose just enough details on each topic for you to get a good idea of the picture and an understanding of of tools and libraries will work well for your particular use case.

Skip to content

Specifically, this lesson covers:

- Tools for efficiently storing data and writing/reading it to/from disk
- Interfacing with databases and object storage solutions
- Main libraries to work with arrays and tabular data
- Performance monitoring and benchmarking
- Workload parallelisation: threads and Dask

See also

> ⚠ Credit
>
> Don't forget to check out additional course materials from the Data carpentry, such as:
>
> - Data Analysis and Visualization in Python for Ecologists
> - 10 minutes to pandas
> - Modern Pandas (blog series by Tom Augspurger)
>
> Moreover, the Polars documentation and Awesome data science with Python are valuable resources, as well as PythonSpeed.

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