DuckDQ

Data Quality Validation for Machine Learning Pipelines

- Introduction
- 3 key design choices behind DuckDQ
- Experiments
- Conclusion

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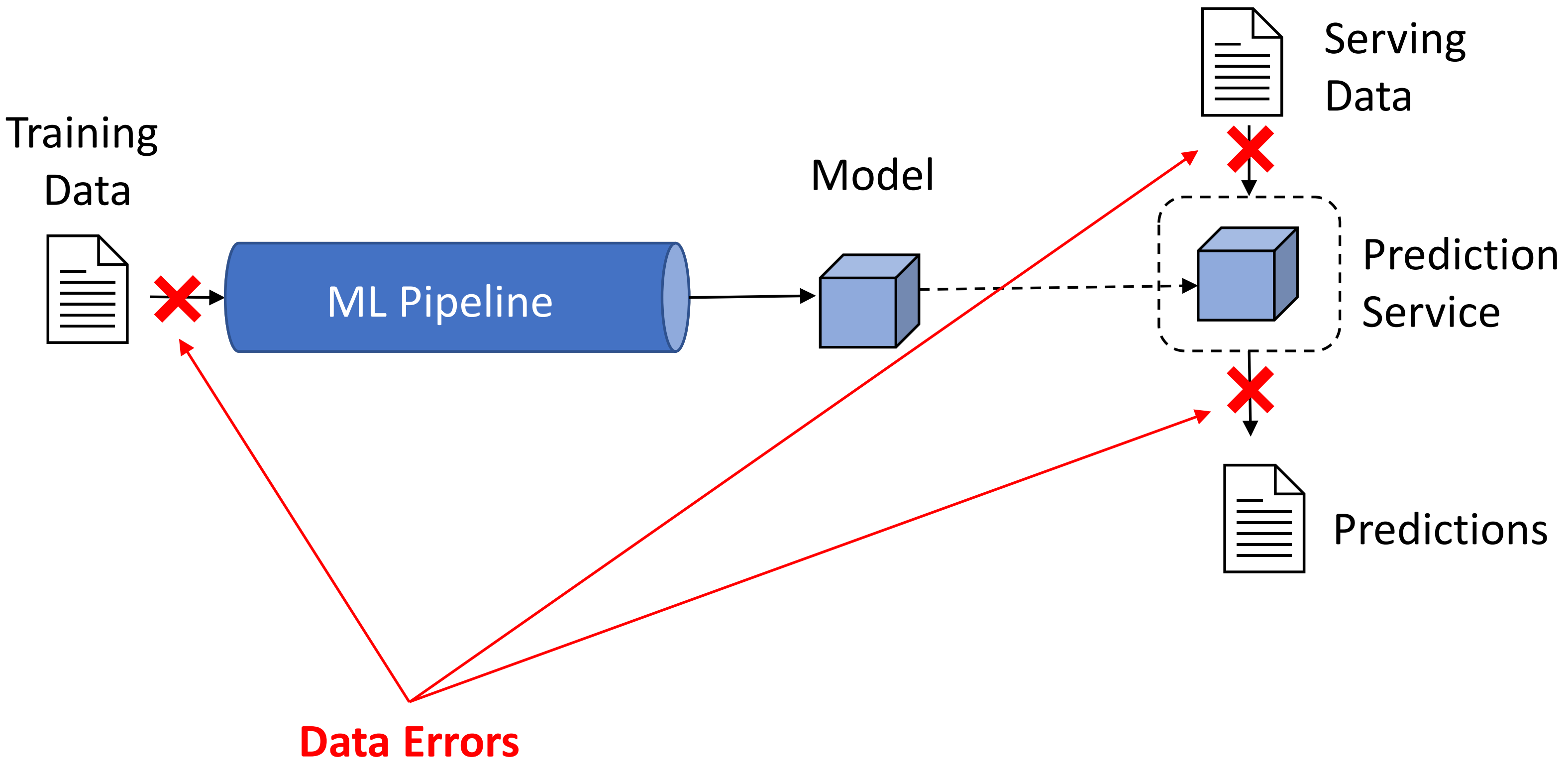
Machine Learning (ML) Pipelines



Data Quality Validation in Python

- Deequ (Apache Spark) [1]
- TFX Data Validation (TensorFlow) [2]
- Great Expectations (pandas + SQL) [3]
- Hooqu (pandas) [4]

```
import com.amazon.deequ.VerificationSuite
import com.amazon.deequ.checks.{Check, CheckLevel, CheckStatus}


val verificationResult = VerificationSuite()
  .onData(data) // spark data frame
  .addCheck(
    Check(CheckLevel.Error, "unit testing my data")
      .hasPattern("date_time",  "(\\d{4}-\\d{2}-\\d{2} \\d{2}:\\d{2}:\\d{2})") // check date format
      .isPositive("trip_distance") // positive trip distance
      .hasApproxQuantile("id", 0.5, _ <= expected_dist()) // check median trip distance via external function
    .run()
```

Deequ Verification API: Code Example

[1] Schelter, Sebastian et al. “Deequ - Data Quality Validation for Machine Learning Pipelines.” : 3.
[2] Polyzotis, Neoklis, et al. "Data validation for machine learning." Proceedings of Machine Learning and Systems 1 (2019): 334-347.
[3] “Home | Great Expectations.” https://greatexpectations.io/ .
[4] “GitHub | mfcabrera/hooqu.” https://github.com/mfcabrera/hooqu .

Data Quality Validation in Python

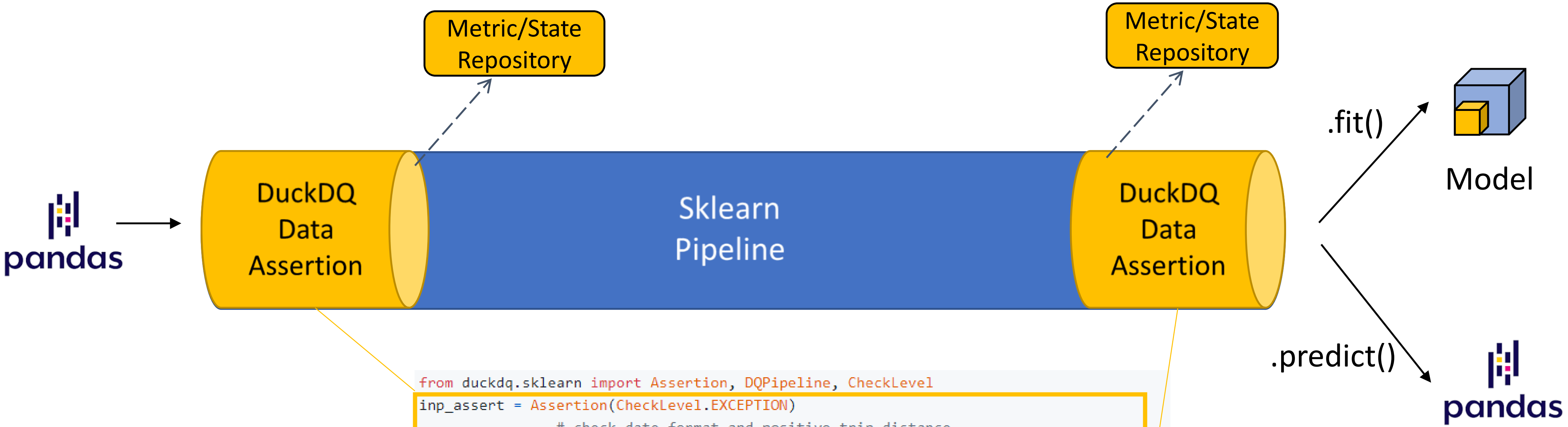
Data Quality Validation for ML in Python:

- either designed for **very large datasets,**
- or tightly coupled to **ML platforms,**
- or lightweight but **not integrated with the ML lifecycle** and (potentially) not optimized for production use.

DuckDQ offers…

- "**Data Assertions**" that can be serialized together with ML models and shipped into production seamlessly.
- **Efficient integration with Pandas** and scikit-learn pipelines.
- **Opportunities for failure analysis and drift detection** even when the original data is not around anymore.
- A flexible, SQL-based computational backend which is also suitable for **efficient validation of data in other SQL databases.**

What are Data Assertions?



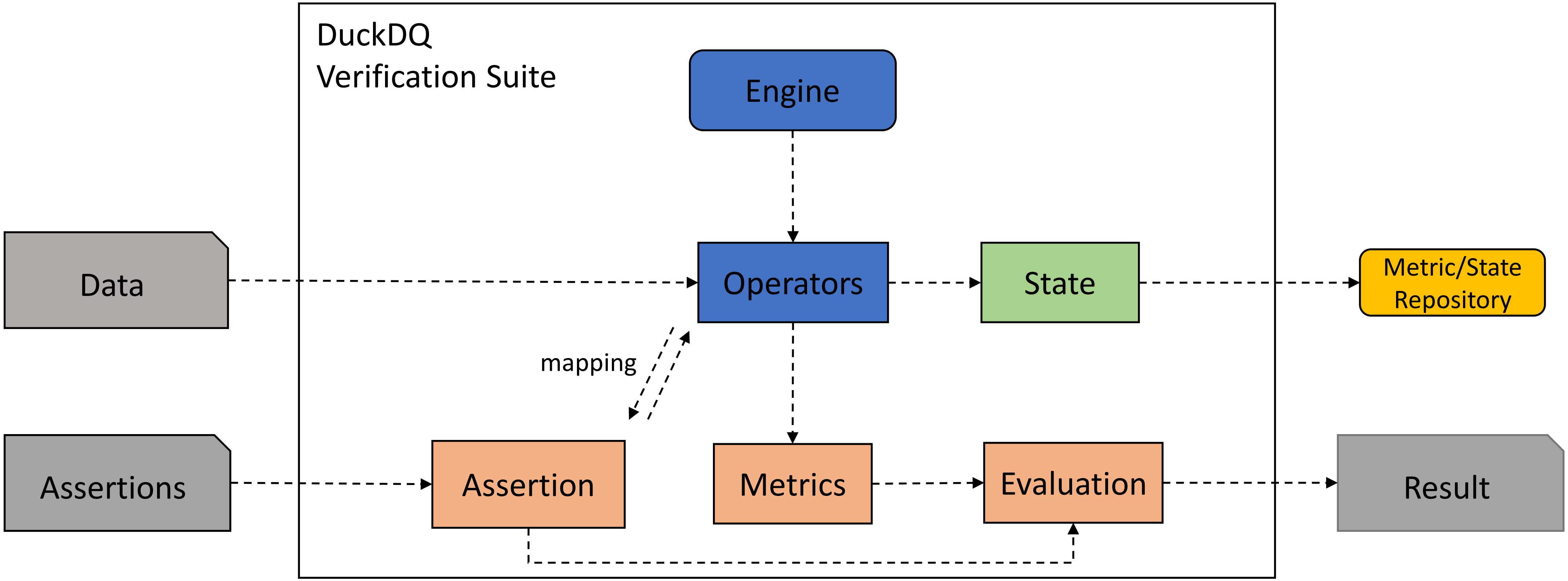

```python
from duckdq.sklearn import Assertion, DQPipeline, CheckLevel
inp_assert = Assertion(CheckLevel.EXCEPTION)
                # check date format and positive trip distance
                .has_pattern("date_time",  r"(\d{4}-\d{2}-\d{2} \d{2}:\d{2}:\d{2})")
                .is_positive("trip_distance")
                # check median trip distance via external function
                .has_quantile("trip_distance",  0.5, lambda x: x <= expected_dist())
outp_assert = Assertion(CheckLevel.WARNING)
                # check ratio of positives is less than 10%
                .has_histogram_values("y",lambda x: x["1"].ratio < 0.1)
pipeline = DQPipeline([
                        ('feature_encoding', Pipeline(...))
                        ('clf', RandomForestClassifier())],
                        input_assertion=inp_assert,
                        output_assertion=outp_assert)
model = pipeline.fit(X_train, y_train)
```

DuckDQ Assertion API: Code Example

Under the Hood…

- Stateful computation of metrics
- Scan sharing optimization
- Integration with DuckDB

Overview



DuckDQ
Verification Suite
Engine
Data
Operators
State
Metric/State
Repository
mapping
Assertions
Assertion
Metrics
Evaluation
Result

Stateful Computation of Metrics

- States are **intermediate representations of metrics**, which **can be merged across multiple batches** of data.

Examples:

Minimum

- States: min
- Merge: minC = min(minA,minB)
- Metric: minC

Mean

- States: total, count
- Merge: totalC = totalA+totalB, countC = countA+countB
- Metric: mean = totalC/countC

Standard Deviation

- States: mean, n, dsq
- Merge:
  - nC = nA + nB
  - avgC = (nA * meanA + nB * meanB) / nC
  - delta = nA - nB
  - dsqC = dsqA + dsqB + delta^2 * nA * nB / nC
- Metric: stddev = sqrt(dsqC / (nC - 1))

data $d \in D$, state s, metric m

Commutative monoid:

$(S, \bigoplus, 0)$

Addition function:

$\bigoplus : S \times S \rightarrow S$

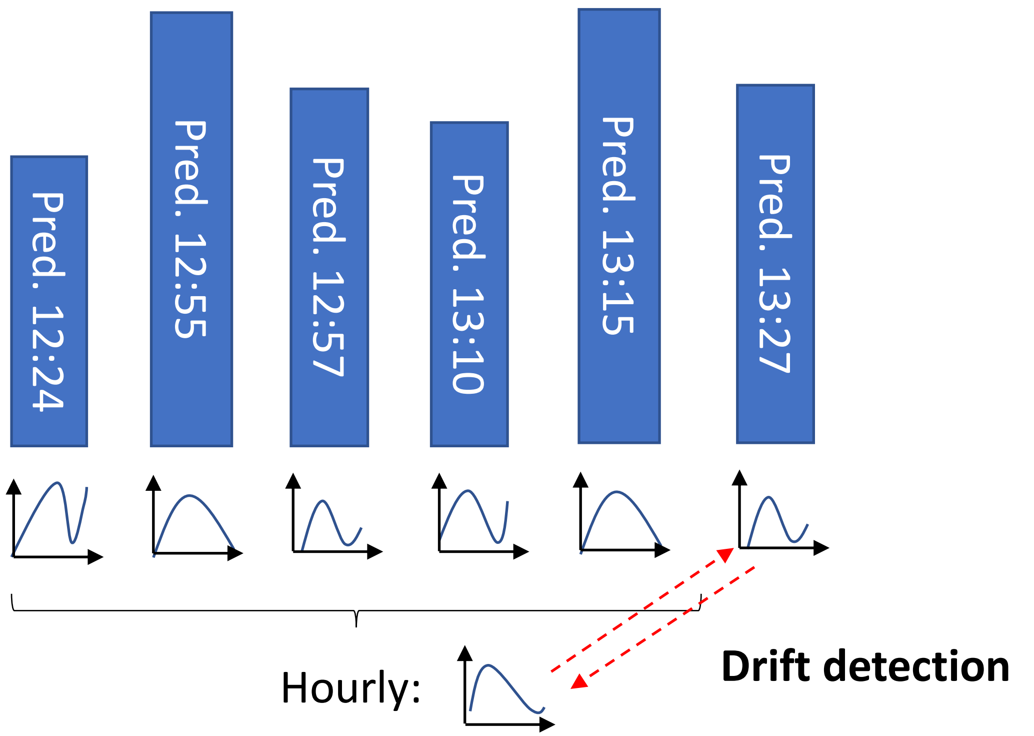
Incremental metrics computation:

$m(s(d1 \cup d2)) = m(s(d1) \bigoplus s(d2))$

- What we call „stateful computations“ are basically streaming/online algorithms
- DataSketches[1] such as KLL (approx. quantiles) and HyperLogLog (approx. distinctness) fit in well with this paradigm.

[1] https://datasketches.apache.org/

Stateful Metrics in the ML Pipelines Context



- States are recorded in every prediction run
- All metics can be merged across multiple prediction batches
- Enables, e.g., drift detection **without processing the data twice / needing to keep the original data around at all**.

Scan Sharing (SQL Engine)

Operators/Assertions

- Minimum
- Maximum
- Mean
- Sum
- StandardDeviation
- Completeness
- Uniqueness
- Distinctness
- HistogramProperty
- ApproxQuantile
- PatternMatch
- MaxLength
- MinLength
- …

- DuckDQ‘s default engine is SQL-based
- Most operators require only a SELECT-statements (blue)
- Some require an additional GROUP BY-statement (black)

Scan Sharing (SQL Engine)

- Instead of executing each operator individually, we group all possible operators into a single query, which requires **only one full table scan** at max (scan sharing).

```
SELECT count(..), sum(..) FROM dataframe
SELECT count(*), count(..) FROM dataframe
SELECT min(..) FROM dataframe
```

```
SELECT count(..), sum(..), count(*), count(..), min(..) FROM dataframe
```

- For GROUP BY-Operators, scan sharing is done as well, but scans can only be shared among operators which require the same groupings.

Integration with DuckDB

„But in the context of Python-based ML Pipelines, we are dealing with DataFrames, so what‘s the use of an SQL engine??“

- That‘s where DuckDB comes in…
- DuckDB is an efficient, in-process analytical RDBMS with a neat Python integration.
- Pandas DataFrames can be queried by the DuckDB engine similar to physical tables.

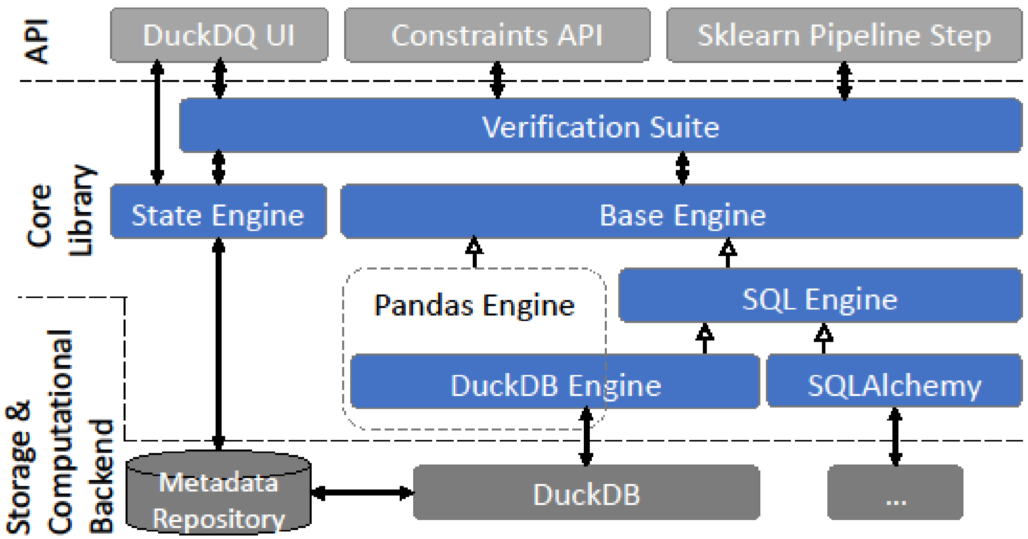
```
import duckdq
import pandas as pd

hotel_search_logs = pd.read_csv (“hotel_search_logs.csv")

count = duckdb.query(“SELECT count(*) FROM hotel_search_logs").fetchone()
print(count)
```

Query a Pandas DataFrame with DuckDB[1]

[1] https://duckdb.org/2021/05/14/sql-on-pandas.html, Raasveldt, Mark, and Hannes Mühleisen. "Efficient SQL on Pandas with DuckDB" *Proceedings of the 2019 International Conference on Management of Data*. 2019.

Integration with DuckDB

- **We can hence apply our SQL-based optimization to Pandas DataFrames.**

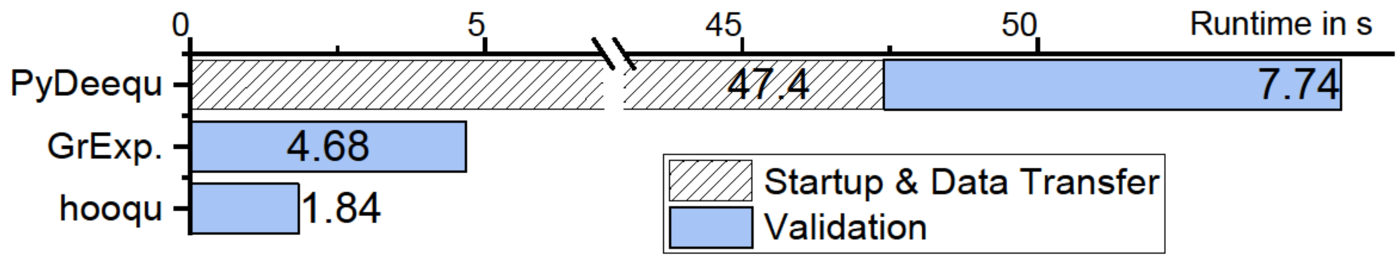


As a side-effect, we can practically use the same SQL engine for general purpose data quality validation on other SQL-based databases.

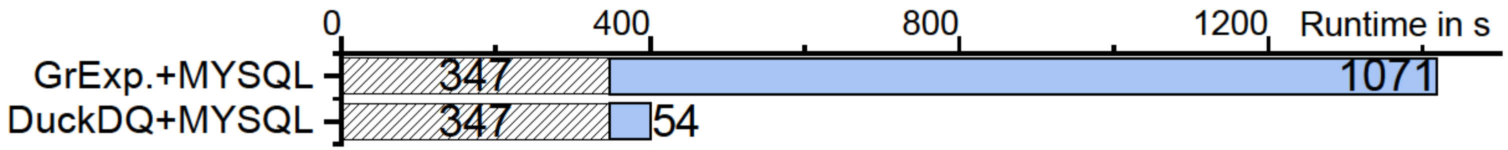
Evaluation

Tests for *completeness* of 5 cols (4 numeric, one string) and *uniqueness* of 5 cols (4 numeric, one string)

A Pandas DataFrame with 3M rows https://www.kaggle.com/c/expedia-hotel-recommendations/data

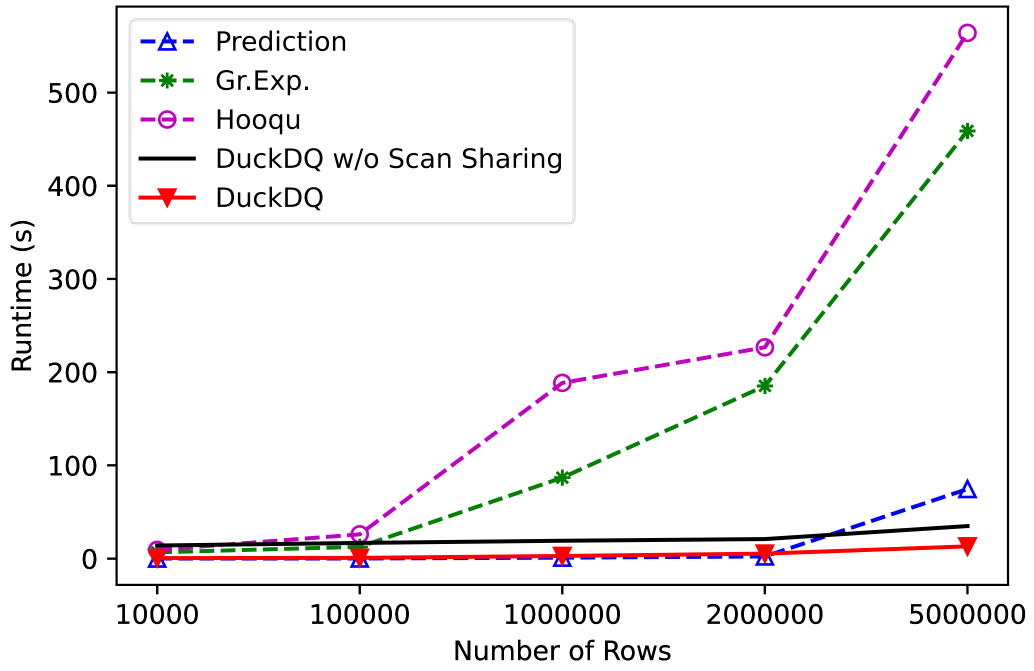


Loading the same data into MYSQL and check the same quality constraints…

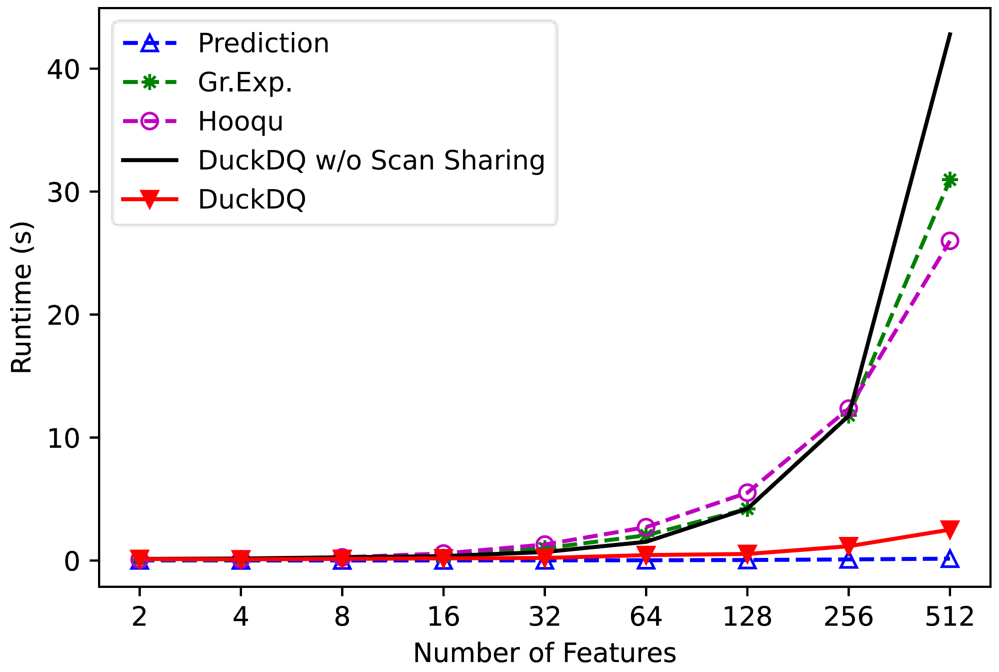


Evaluation

- Is the difference relevant?
- Let's put the validation time is relation to the prediction time across different data set sizes..



with varying number of rows



with varying number of features

Conclusion

- Current solutions for DQA in the Python data science ecosystem pose a potential runtime bottleneck in ML pipelines.
- DuckDQ:
  - is a lightweight and efficient solution for keeping ML pipelines error-free which does not require any heavy additional infrastructure.
  - It is particularly well suited for medium-sized data sets.
  - Offers opportunities for ML-monitoring (e.g. drift detection).
- Lowering the entry barrier for the adoption of MLOps best practices.

More about DuckDQ…

- Source Code: https://github.com/tdoehmen/duckdq
- Publication: Till Döhmen, Mark Raasveldt, Hannes Mühleisen, Sebastian Schelter “DuckDQ: Data Quality Assertions for Machine Learning Pipelines” ICML 2021 Workshop – Challenges in Deploying and Monitoring Machine Learning Systems