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Best Practices in Pandas

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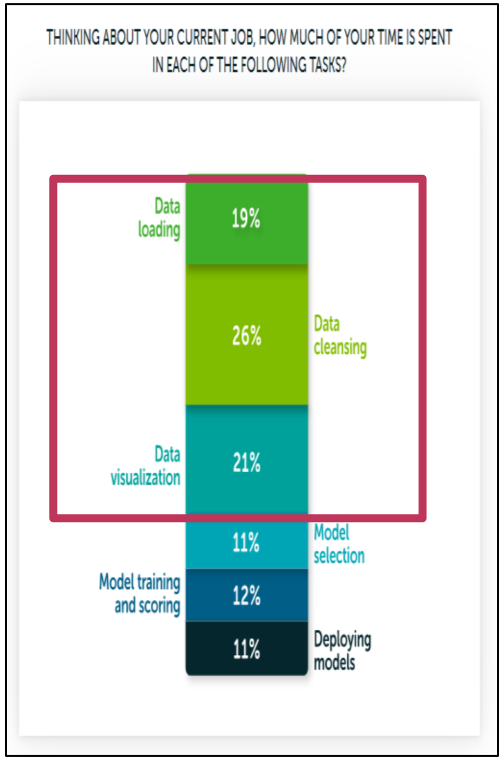
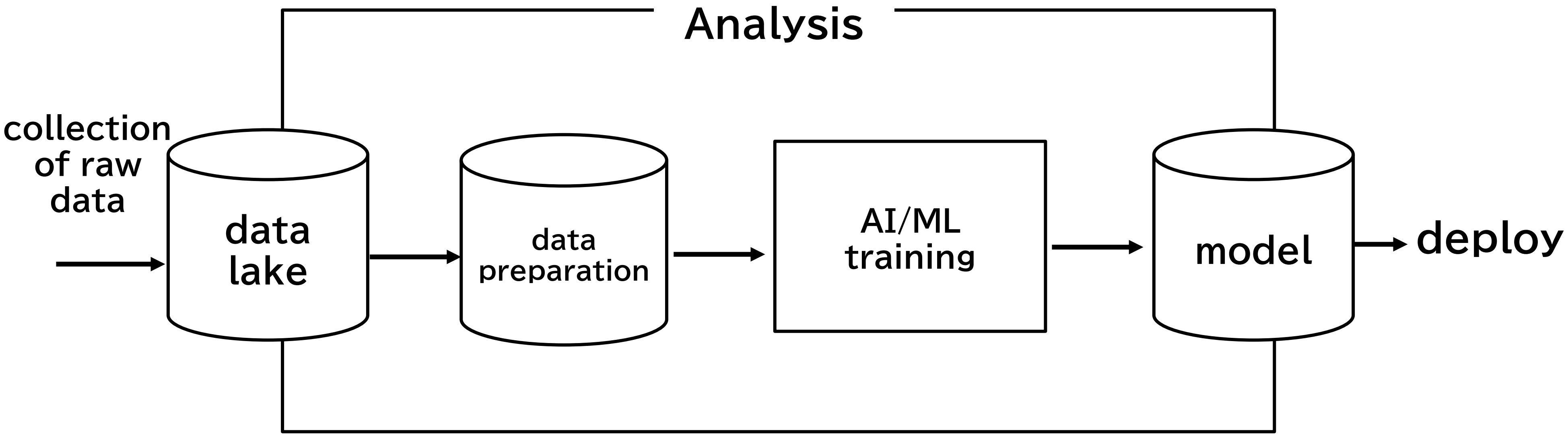
Workflow of a Data Scientist

almost 75% efforts of a Data Scientist spent on data preparation

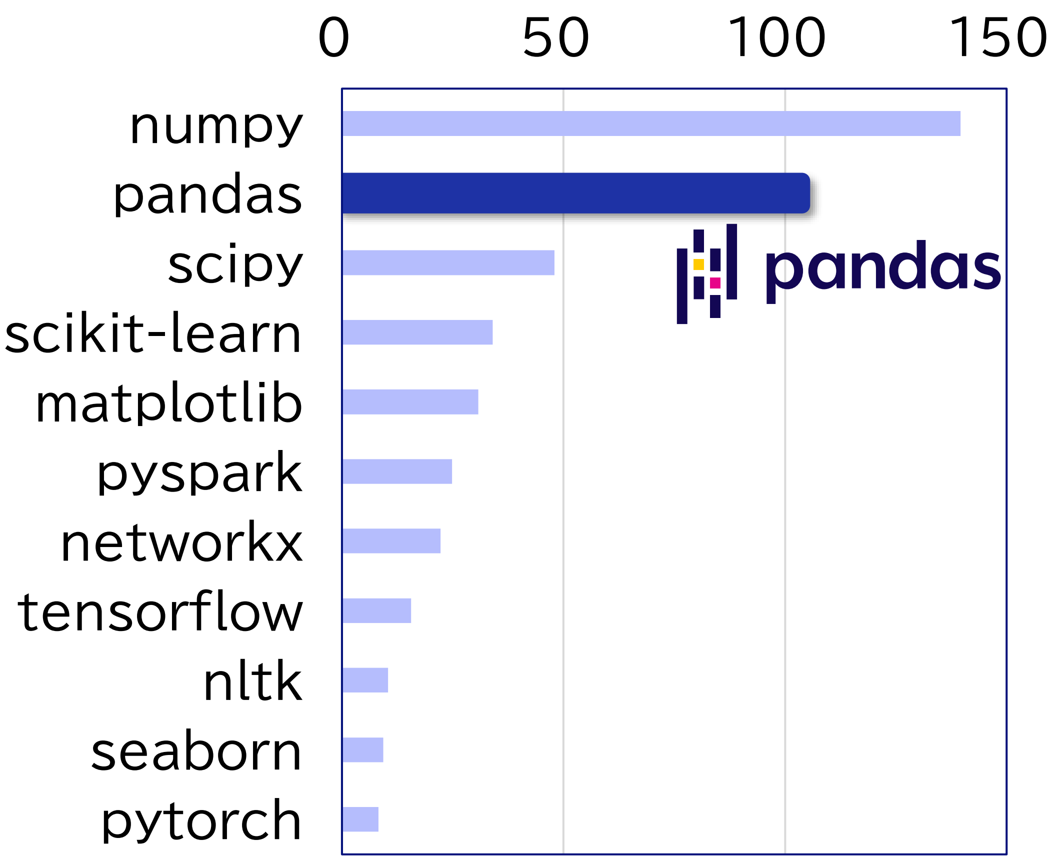


Anaconda:
The State of Data Science 2020



About Pandas

◆ **Most popular Python library for data analytics.**



Monthly download from pypi.org
(Data Analytics Libraries)

The way of implementing a query in pandas-like library (that does not support query optimization) heavily impacts its performance!!

- We will discuss a couple of approaches to improve the performance related to computational time and memory of a query written in pandas, when processing large-scale data.
- We will also discuss how those approaches can be automated.

Best Practices

(1) importance of chained expression

```
def foo(filename):
  df = pd.read_csv(filename)
  t1 = df.drop_duplicates()
  t2 = t1[t1[“B”] > 0.20]
  t3 = t2.sort_values(“B”)
  t4 = t3.head(2)
  return t4
```

df: ~16 GB

A	B	C
u	0.91	1
a	1.00	4
a	1.00	4
o	0.24	0
o	0.24	0
e	0.43	1
u	0.91	1
e	0.20	2
o	0.24	0
a	1.00	4

drop_duplicates

t1: ~8 GB

A	B	C
u	0.91	1
a	1.00	4
o	0.24	0
e	0.43	1
e	0.20	2

filter

t2: ~8 GB

A	B	C
u	0.91	1
a	1.00	4
o	0.24	0
e	0.43	1

sort

t3: ~8 GB

A	B	C
a	1.00	4
u	0.91	1
e	0.43	1
o	0.24	0

head(2)

t4: ~x KB

A	B	C
a	1.00	4
u	0.91	1

re-write using chained expression

```
def foo(filename):
  return (
    pd.read_csv(filename)
      .drop_duplicates()
      .??
      .sort_values(“B”)
      .head(2)
  )
```

```
def foo(filename):
  return (
    pd.read_csv(filename)
      .drop_duplicates()
      .query(“B > 0.20”)
      .sort_values(“B”)
      .head(2)
  )
```

query(): allows you to write SQL-like conditional expression, helping you to perform filter on the current state of the input frame, but its a little slower as it parses the input string to construct the filter mask.

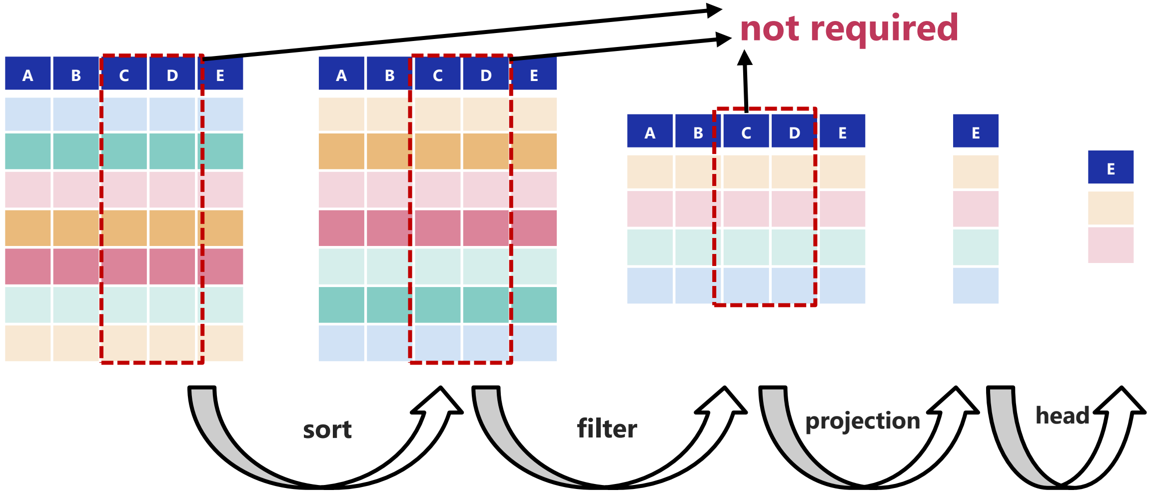
```
def foo(filename):
  return (
    pd.read_csv(filename)
      .drop_duplicates()
      .pipe(lambda tmp: tmp[tmp[“B”] > 0.20]
      .sort_values(“B”)
      .head(2)
  )
```

pipe(): a convenient method allowing you to perform a given operation (like filter etc.) on the current state of the input frame without introducing computational overhead.

(2) importance of execution order

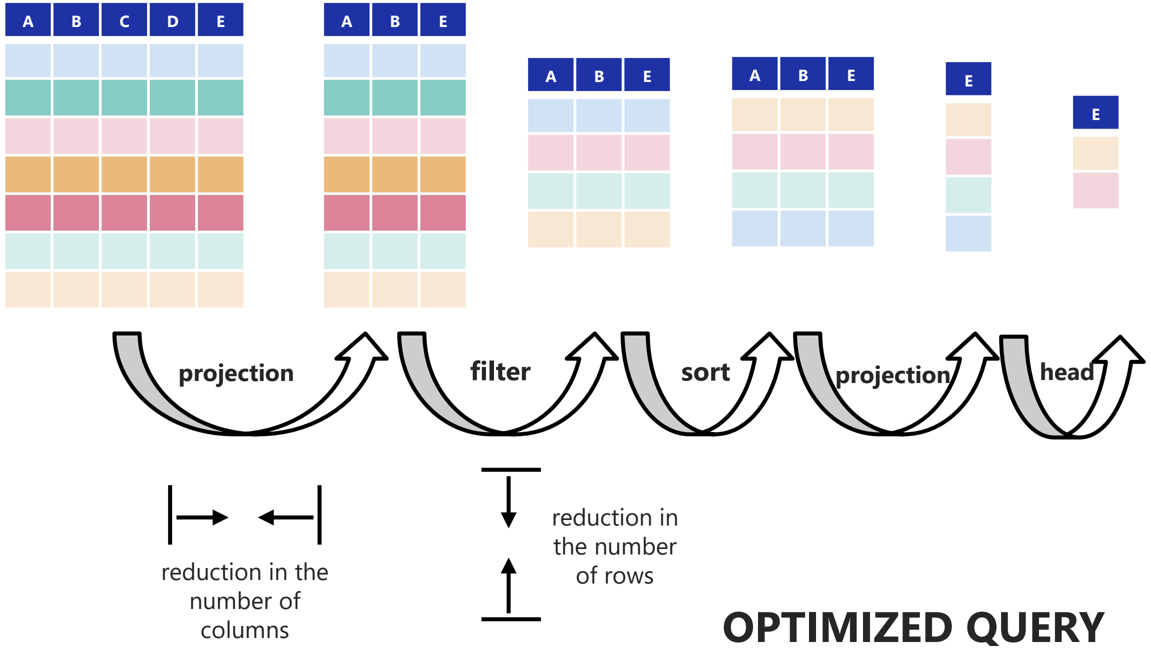
```
df.sort_values("A")
  .query("B > 1")["E"]
  .head(2)
```

※sort-order: yellow->red->green->blue
※B=1for darker shade, B=2 for lighter shade



SAMPLE QUERY

```
df.loc[:, ["A", "B", "E"]]
  .query("B > 1")
  .sort_values("A")["E"]
  .head(2)
```

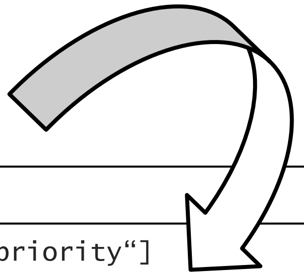


OPTIMIZED QUERY

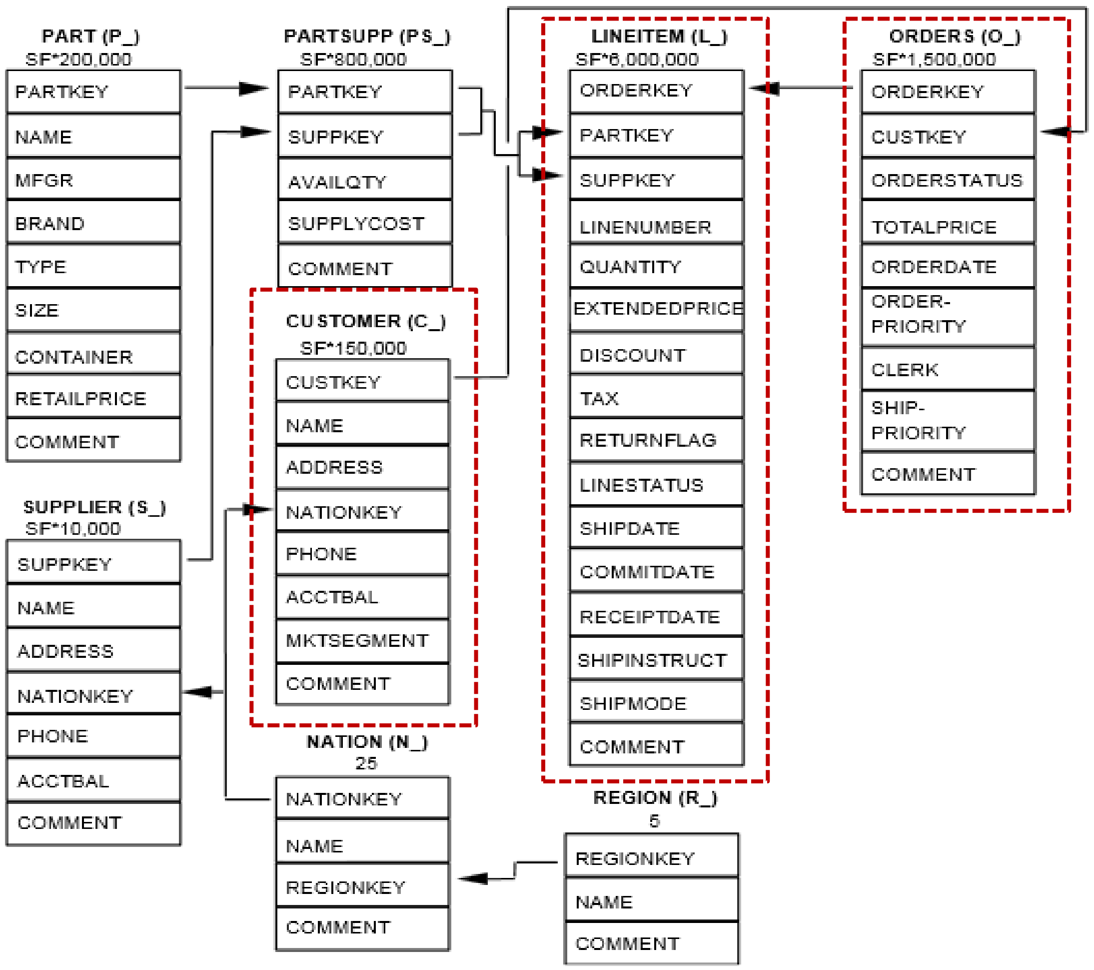
Exercise: Query #3 from TPC-H Benchmark (SQL -> pandas)

◆ [query to retrieve the 10 unshipped orders with the highest value.]()

```
SELECT l_orderkey,
               sum(l_extendedprice * (1 - l_discount)) as revenue,
               o_orderdate,
               o_shippriority
FROM customer, orders, lineitem
WHERE
    c_mktsegment = 'BUILDING' AND
    c_custkey = o_custkey AND
    l_orderkey = o_orderkey AND
    o_orderdate < date '1995-03-15' AND
    l_shipdate > date '1995-03-15'
GROUP BY l_orderkey, o_orderdate, o_shippriority
ORDER BY revenue desc, o_orderdate
LIMIT 10;
```

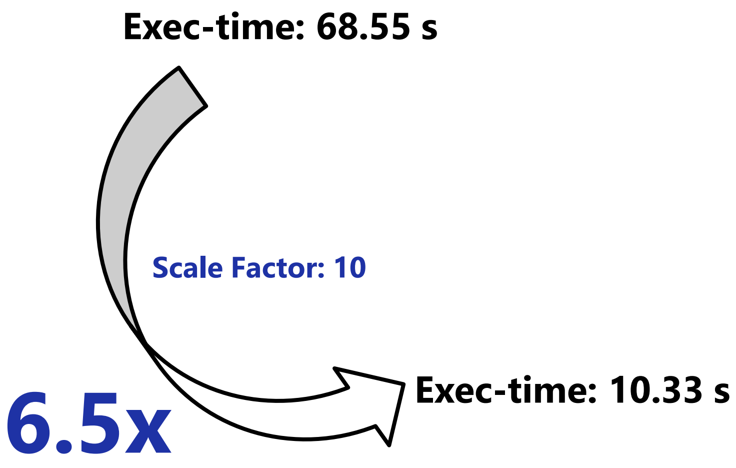


```
rescols = ["l_orderkey", "revenue", "o_orderdate", "o_shippriority"]
result = (
 customer.merge(orders, left_on="c_custkey", right_on="o_custkey")
  .merge(lineitem, left_on="o_orderkey", right_on="l_orderkey")
  .pipe(lambda df: df[df["c_mktsegment"] == "BUILDING"])
  .pipe(lambda df: df[df["o_orderdate"] < datetime(1995, 3, 15)])
  .pipe(lambda df: df[df["l_shipdate"] > datetime(1995, 3, 15)])
  .assign(revenue=lambda df: df["l_extendedprice"] * (1 - df["l_discount"]))
  .groupby(["l_orderkey", "o_orderdate", "o_shippriority"], as_index=False)
  .agg({"revenue": "sum"})[rescols]
  .sort_values(["revenue", "o_orderdate"], ascending=[False, True])
  .head(10)
)
```



Exercise: Query #3 from TPC-H Benchmark (pandas -> optimized pandas)

```
rescols = ["l_orderkey", “revenue”, "o_orderdate", "o_shippriority“]
result = (
 customer.merge(orders, left_on="c_custkey", right_on="o_custkey")
  .merge(lineitem, left_on="o_orderkey", right_on="l_orderkey")
  .pipe(lambda df: df[df[“c_mktsegment"] == "BUILDING"])
  .pipe(lambda df: df[df["o_orderdate"] < datetime(1995, 3, 15)])
  .pipe(lambda df: df[df["l_shipdate"] > datetime(1995, 3, 15)])
  .assign(revenue=lambda df: df["l_extendedprice"] * (1 - df["l_discount"]))
  .groupby(["l_orderkey", "o_orderdate", "o_shippriority"], as_index=False)
  .agg({"revenue": "sum”})[rescols]
  .sort_values(["revenue", "o_orderdate"], ascending=[False, True])
  .head(10)
)
```



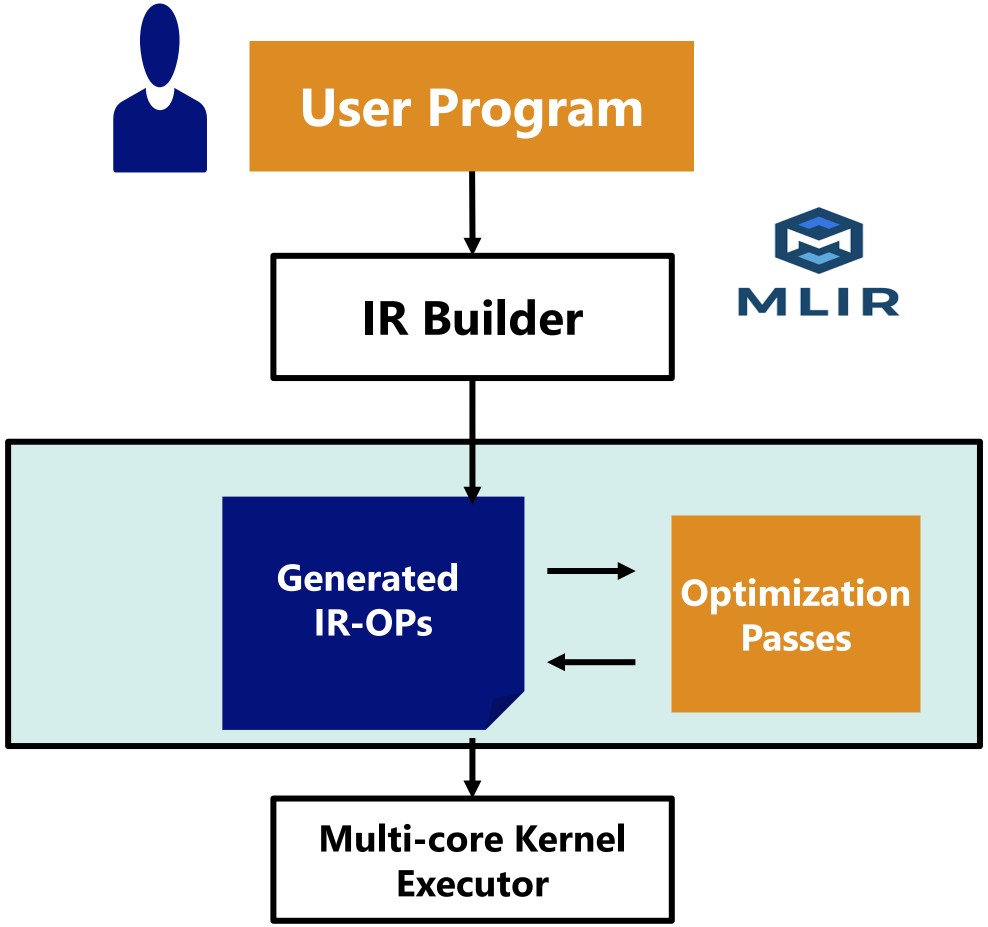

```
# projection-filter: to reduce scope of “customer” table to be processed
cust = customer[[“c_custkey”, “c_mktsegment”]] # (2/8)
f_cust = cust[cust[“c_mktsegment"] == "BUILDING"]

# projection-filter: to reduce scope of “orders” table to be processe
ord = orders[[“o_custkey”, “o_orderkey”, “o_orderdate”, "o_shippriority"]] (4/9)
f_ord = ord[ord["o_orderdate"] < datetime(1995, 3, 15)]

# projection-filter: to reduce scope of “lineitem” table to be processed
litem = lineitem[["l_orderkey“, "l_shipdate“, "l_extendedprice“, "l_discount"]] (4/16)
f_litem = litem[litem["l_shipdate"] > datetime(1995, 3, 15)]

rescols = ["l_orderkey", “revenue”, "o_orderdate", "o_shippriority“]
result = ( f_cust.merge(f_ord, left_on="c_custkey", right_on="o_custkey")
  .merge(f_litem, left_on="o_orderkey", right_on="l_orderkey")
  .assign(revenue=lambda df: df["l_extendedprice"] * (1 - df["l_discount"]))
  .pipe(lambda df: df[rescols])
  .groupby(["l_orderkey", "o_orderdate", "o_shippriority"], as_index=False)
  .agg({"revenue": "sum"})[rescols]
  .sort_values(["revenue", "o_orderdate"], ascending=[False, True])
  .head(10)
)
```

Automatic Optimization

Introducing FireDucks

※IR: Intermediate Representation

FireDucks (**F**lexible **IR E**ngine for DataFrame) is a high-performance compiler-accelerated DataFrame library with highly compatible pandas APIs.




```
result = df.sort_values(“A”)
   .query(“B > 1”)[“E”]
   .head(2)
```

```
%v2 = “sort_values_op"(%v1, “A")
%v3 = "filter_op"(%v2, “B > 1”)
%v4 = “project_op”(%v3, [“E”])
%v5 = “slice_op”(%v4, 2)
```

print (result)

```
%t1 = “project_op”(%v1, [“A”, “B”, “E”])
%t2 = "filter_op"(%t1, “B > 1”)
%t3 = “sort_values_op"(%t2, “A")
%t4 = “project_op”(%t3, [“E”])
%t5 = “slice_op”(%t4, 2)
```

```
result = df.loc[:, [“A”, “B”, “E”]]
   .query(“B > 1”)
   .sort_values(“A”)[“E”]
   .head(2)
```

Primary Objective: <u>Write Once, Execute Anywhere</u>

IR-driven Lazy-execution addresses memory issue with intermediate tables

```
def foo(filename):
  df = pd.read_csv(filename)
  t1 = df.drop_duplicates()
  t2 = t1[t1["B"] > 0.20]
  t3 = t2.sort_values("B")
  t4 = t3.head(2)
  return t4

ret = foo("data.csv")
print(ret.shape)
```

example without chained expression

```
def foo(filename):
  return (
    pd.read_csv(filename)
      .drop_duplicates()
      .query("B > 0.20")
      .sort_values("B")
      .head(2)
  )

ret = foo("data.csv")
print(ret.shape)
```

example with chained expression

```
%t3 = read_csv_with_metadata('dummy.csv', ...)
%t4 = drop_duplicates(%t3, ...)
%t5 = project(%t4, 'B')
%t6 = gt.vector.scalar(%t5, 0.20)
%t7 = filter(%t4, %t6)
%t8 = sort_values(%t7, ['B'], [True])
%t9 = slice(%t8, 0, 2, 1)
%v10 = get_shape(%t9)
return(%t9, %v10)
```

IR Generated by FireDucks
(can be inspected when setting environment variable FIRE_LOG_LEVEL=3)

Why FireDucks?

※IR: Intermediate Representation

FireDucks (**F**lexible **IR** **E**ngine for DataFrame) is a high-performance compiler-accelerated DataFrame library with highly compatible pandas APIs.

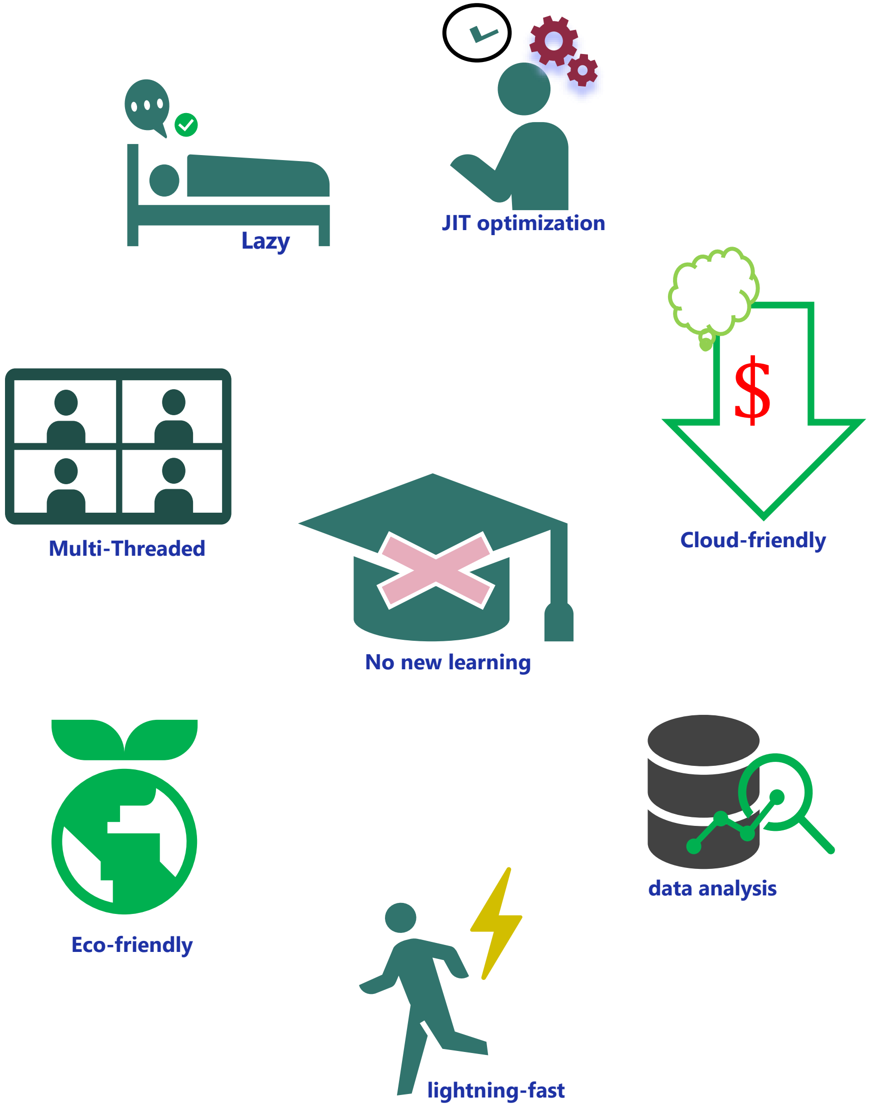
Speed: significantly faster than pandas

- FireDucks is multithreaded to fully exploit the modern processor
- Lazy execution model with Just-In-Time optimization using a defined-by-run mechanism supported by MLIR (a subproject of LLVM).
  - supports both lazy and non-lazy execution models without modifying user programs (same API).

MLIR

Ease of use: drop-in replacement of pandas

- FireDucks is highly compatible with pandas API
  - seamless integration is possible not only for an existing pandas program but also for any external libraries (like seaborn, scikit-learn, etc.) that internally use pandas dataframes.
- No extra learning is required
- No code modification is required



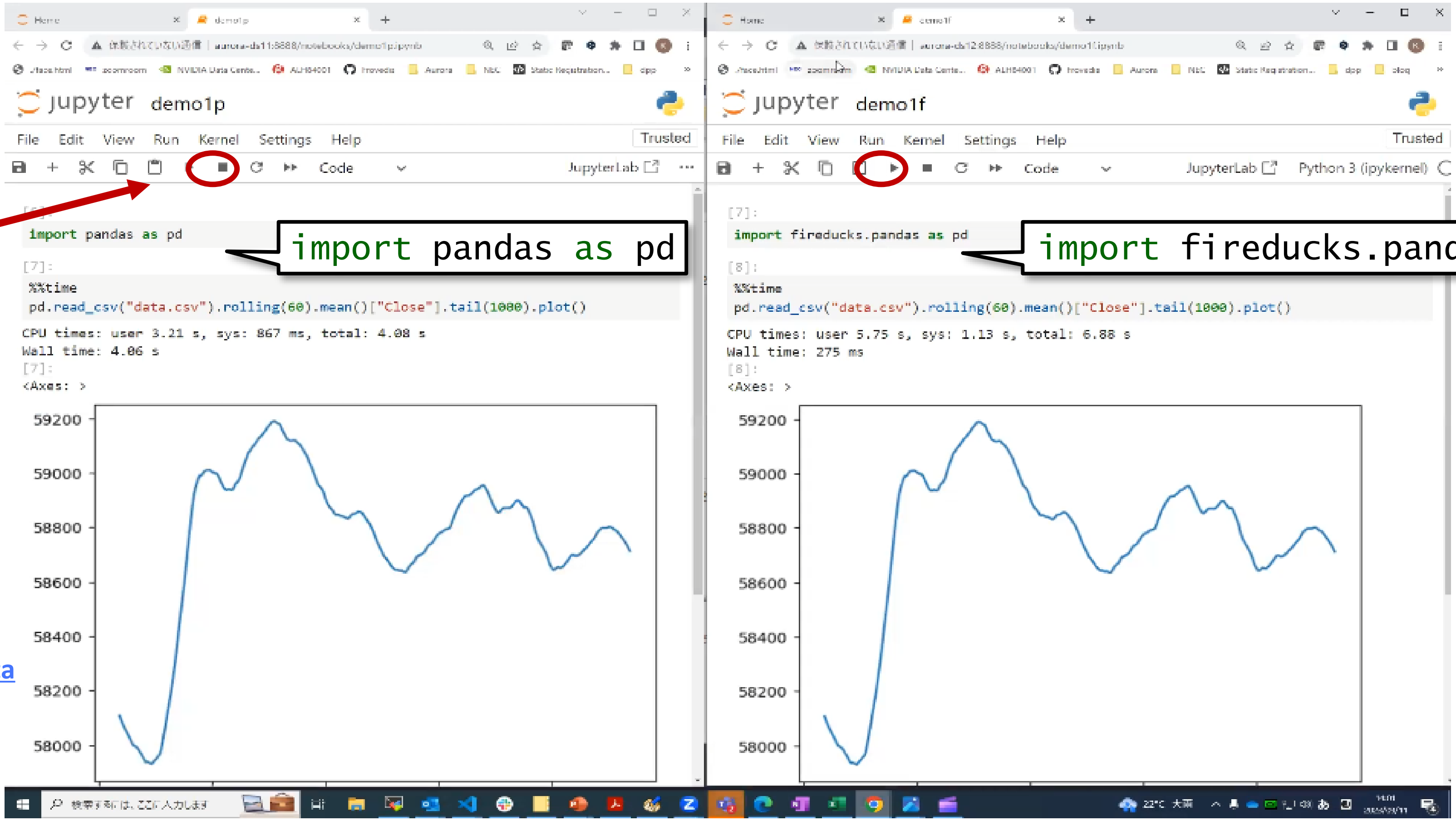
Let's Have a Quick Demo!

```
pd.read_csv("data.csv").rolling(60).mean()["Close"].tail(1000).plot()
```

Program to calculate moving average

pandas the difference is only in the import **FireDucks**

button to start execution



`import pandas as pd`

`import fireducks.pandas as pd`

data.csv: [Bitcoin Historical Data]

pandas: 4.06s

~15x

FireDucks: 275ms

Usage of FireDucks

1. Explicit Import

easy to import

```
# import pandas as pd
import fireducks.pandas as pd
```

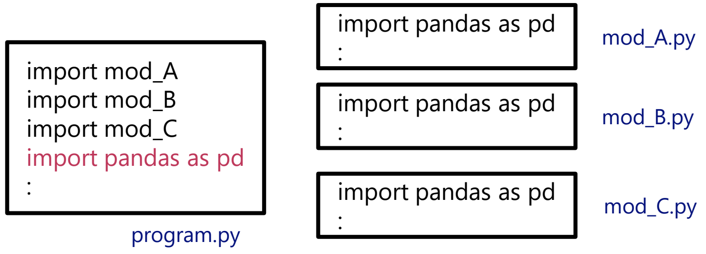
simply change the import statement

2. Import Hook

FireDucks provides command line option to automatically replace “**pandas**” with “**fireducks.pandas**”

```
$ python -m fireducks.pandas program.py
```

zero code modification



3. Notebook Extension

FireDucks provides simple import extension for interative notebooks.

```
%load_ext fireducks.pandas
import pandas as pd
```

simple integration in a notebook

Benchmark (1): DB-Benchmark

Database-like ops benchmark (https://duckdblabs.github.io/db-benchmark)

groupby join

0.5 GB 5 GB 50 GB

basic questions

rank-1

Input table: 1,000,000,000 rows x 9 columns (50 GB)

FireDucks	1.0.4	2024-09-10	15s
DuckDB	1.0.0	2024-07-04	25s
ClickHouse	24.5.1.1763	2024-06-07	28s
Polars	1.1.0	2024-07-09	47s
Datafusion	38.0.1	2024-06-07	56s
data.table	1.15.99	2024-06-07	88s
DataFrames.jl	1.6.1	2024-06-07	91s
InMemoryDatasets	0.7.18	2023-10-17	218s
spark	3.5.1	2024-06-07	261s
R-arrow	16.1.0	2024-06-07	378s
collapse	2.0.14	2024-06-07	411s
(py)datatable	1.2.0a0	2024-06-07	1022s
dplyr	1.1.4	2024-06-07	1104s
pandas	2.2.2	2024-06-07	1126s
dask	2024.5.2	2024-06-07	out of memory
Modin		see README	pending

groupby join

0.5 GB 5 GB 50 GB

basic questions

rank-1

Input table: 100,000,000 rows x 7 columns (5 GB)

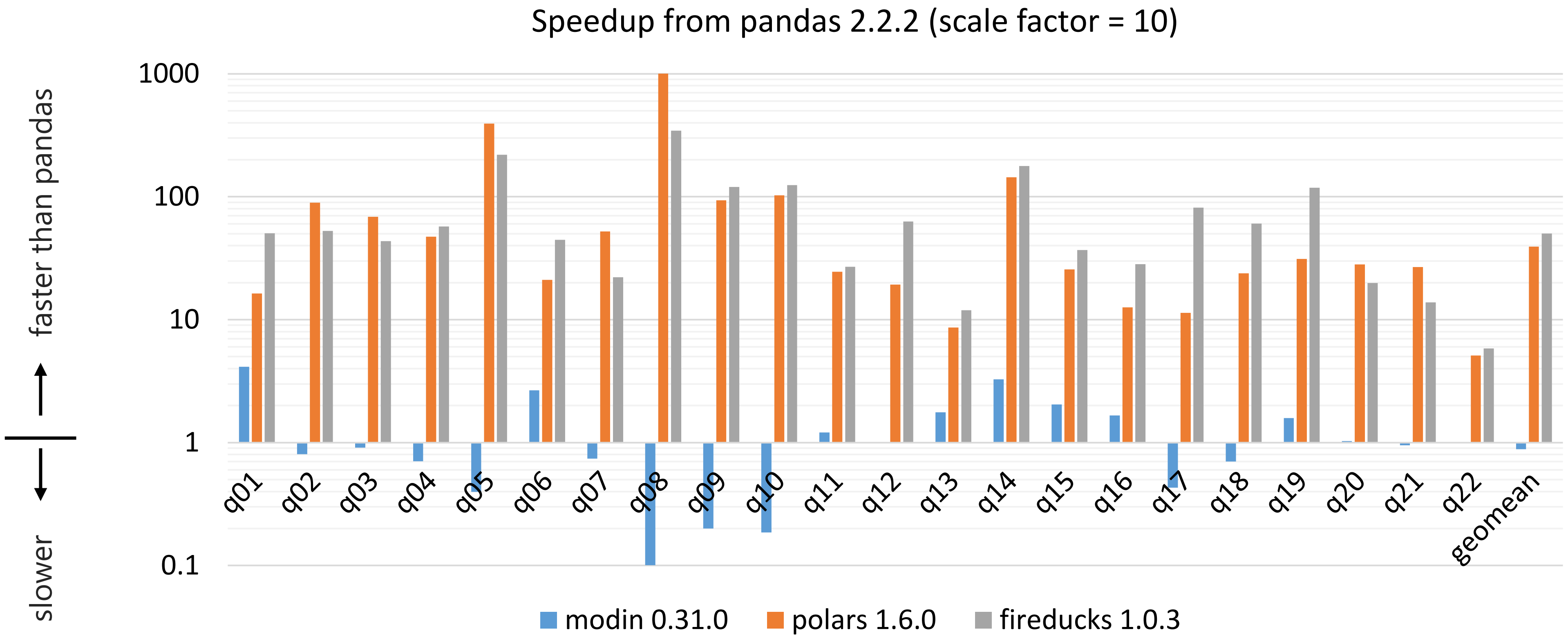
FireDucks	1.0.4	2024-09-10	7s
DuckDB	1.0.0	2024-07-04	9s
Polars	1.1.0	2024-07-08	9s
Datafusion	38.0.1	2024-06-07	15s
InMemoryDatasets	0.7.18	2023-10-20	25s
ClickHouse	24.5.1.1763	2024-06-07	43s
data.table	1.15.99	2024-06-07	62s
collapse	2.0.14	2024-06-07	69s
DataFrames.jl	1.6.1	2024-06-07	77s
spark	3.5.1	2024-06-07	128s
dplyr	1.1.4	2024-06-07	214s
pandas	2.2.2	2024-06-07	244s
dask	2024.5.2	2024-06-07	635s
(py)datatable	1.2.0a0	2024-06-07	undefined exception
R-arrow	16.1.0	2024-06-07	out of memory
Modin		see README	pending

Benchmark (2): Speedup from pandas in TPC-H benchmark

Server

Xeon Gold 5317 x2 (24 cores), 256GB

FireDucks is ~345x faster than pandas at max

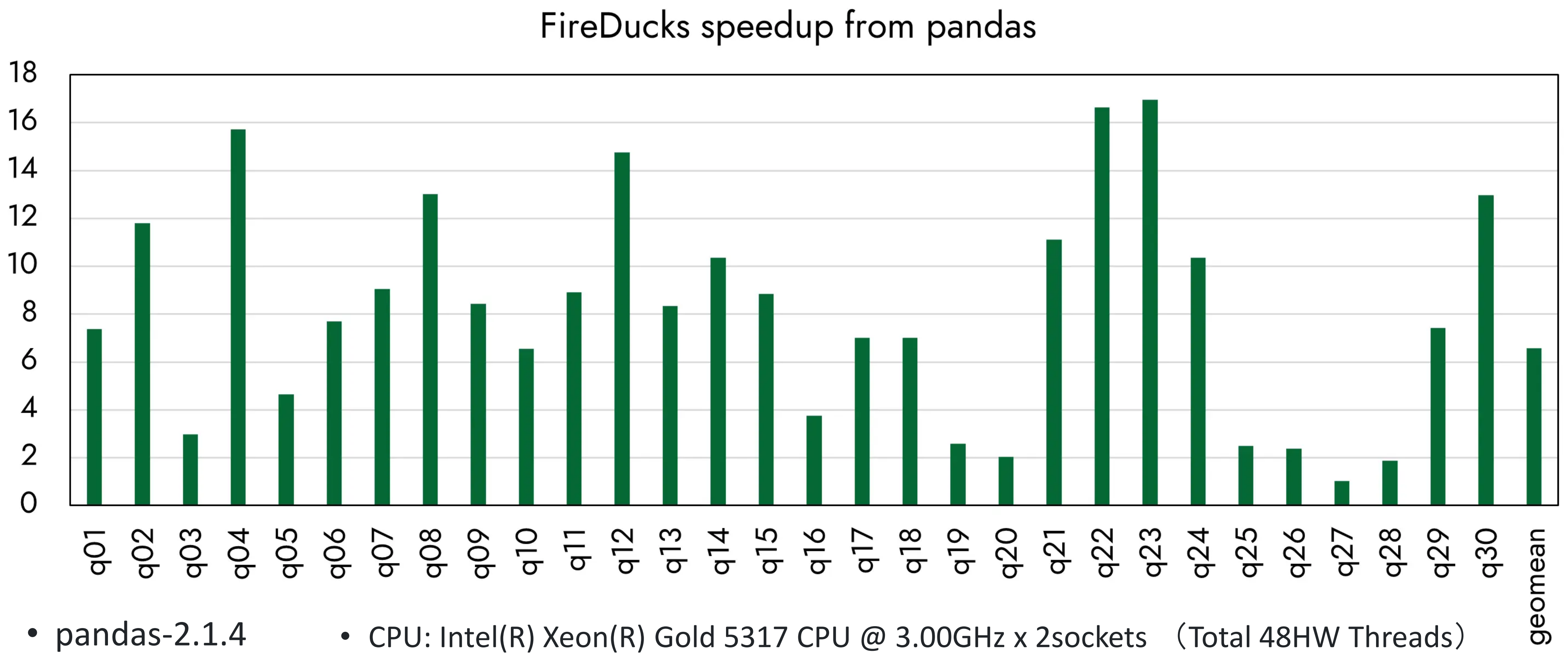


Comparison of DataFrame libraries (average speedup)

FireDucks	**50x**
Polars	39x
Modin	0.9x

Benchmark (3): Speedup from pandas in TPCx-BB benchmark

ETL(Extract, Transform, Load) and ML Workflow



- pandas-2.1.4
- fireducks-0.9.3

- CPU: Intel(R) Xeon(R) Gold 5317 CPU @ 3.00GHz x 2sockets （Total 48HW Threads）
- Main memory: 256GB

Resource on FireDucks

Web site (User guide, benchmark, blog)

https://fireducks-dev.github.io/

X(twitter) (Release information)

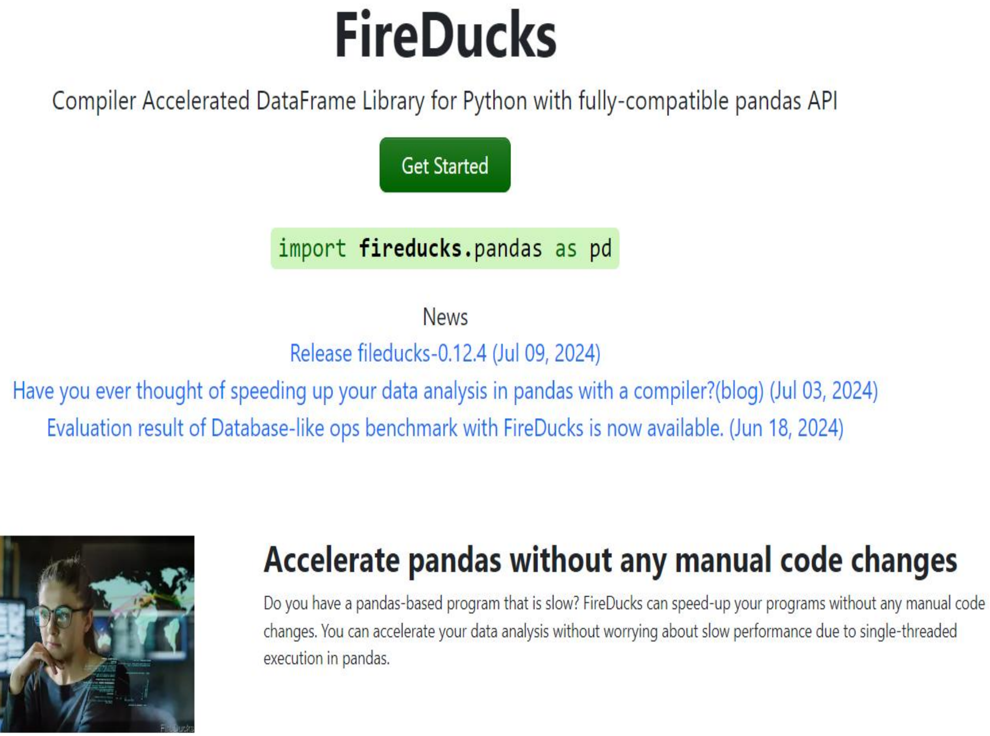
https://x.com/fireducksdev

Github (Issue report)

https://github.com/fireducks-dev/fireducks

slack Q/A, communication

https://join.slack.com/t/fireducks/shared_invite/zt-2j4lucmtj-IGR7AWlXO62Lu605pnBJ2w



Let’s go for a test drive!

https://colab.research.google.com/drive/1qpej-X7CZsIeOqKuhBg4kq-cbGuJf1Zp?usp=sharing

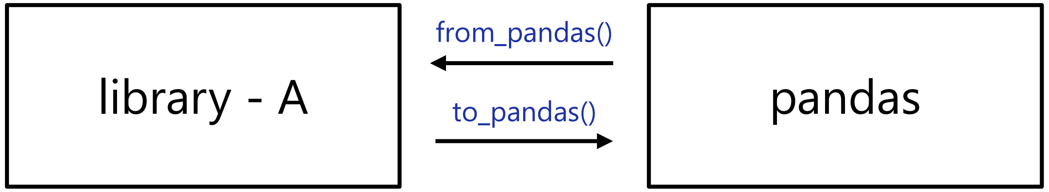
Thank You!

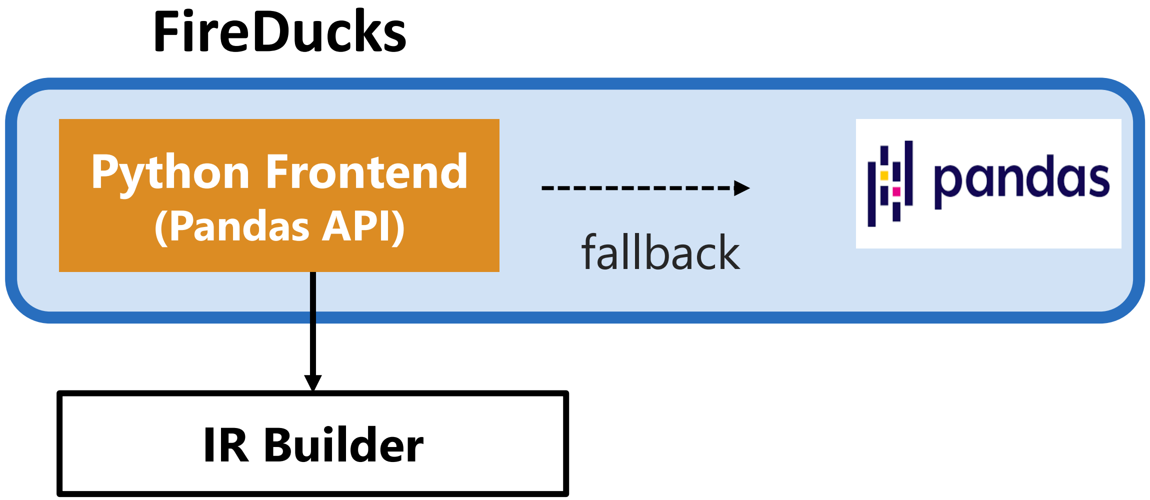
- Focus more on in-depth data exploration using “**pandas**”.
- Let the “**FireDucks**” take care of the optimization for you.
- Enjoy Green Computing!

https://www.linkedin.com/in/sourav-%E3%82%BD%E3%82%A6%E3%83%A9%E3%83%96-saha-%E3%82%B5%E3%83%8F-a5750259/
https://twitter.com/SouravSaha97589

Frequently Asked Questions

FAQ: Why FireDucks is highly compatible with pandas?






```
%load_ext fireducks.pandas    ← notebook extension for importhook
import pandas as pd
import numpy as np
```

```
%%fireducks.profile           ← notebook specific profiler
df = pd.DataFrame({
    "id": np.random.choice(list("abcdef"), 10000),
    "val": np.random.choice(100, 10000)
})

r1 =(
    df.sort_values("id")
      .groupby("id")
      .head(2)
      .reset_index(drop=True)
)
                pd.from_pandas(r1["val"].to_pandas().cumsum())
r1["val"] = r1["val"].cumsum()
r1.describe()
```

profiling-summary:: total: 42.4832 msec (fallback: 1.1448 msec)

	name	type	n_calls	duration (msec)
0	groupby_head	kernel	1	16.696805
1	sort_values	kernel	1	16.684564
2	from_pandas.frame.metadata	kernel	2	3.641694
3	to_pandas.frame.metadata	kernel	2	2.237987
4	describe	kernel	1	2.021135
5	DataFrame._repr_html_	fallback	1	1.021662
6	Series.cumsum	fallback	1	0.111802
7	setitem	kernel	1	0.010280
8	get_metadata	kernel	1	0.009650
9	reset_index	kernel	1	0.008050

When running a python script/program, you may like to set the environment variable to get fallback warning logs:
FIREDUCKS_FLAGS="-Wfallback"

Raise feature request when you encounter some expensive fallback hindering your program performance!

Directly **communicate** with us over our slack channel for any performance or API related queries!

FAQ: How to evaluate Lazy Execution?

```
def foo(employee, country):
    stime = time.time()
    m = employee.merge(country, on=“C_Code”)
    r = m[m[“Gender”] == “Male”]
    print(f”fireducks time: {time.time() – stime} sec”)
    return r
```

IR Builder

create_data_op(…)
merge_op(…)
filter_op(…)

fireducks time: 0.0000123 sec

```
def foo(employee, country):
    employee._evaluate()
    country._evaluate()
    stime = time.time()
    m = employee.merge(country, on=“C_Code”)
    r = m[m[“Gender”] == “Male”]
    r._evaluate()
    print(f”fireducks time: {time.time() – stime} sec”)
    return r
```

fireducks time: 0.02372143 sec

FIREDUCKS_FLAGS="--benchmark-mode”

Use this to disable lazy-execution mode when you do not want to make any changes in your existing application during performance evaluation.

FAQ: How to configure number of cores to be used?

OMP_NUM_THREADS=1

Use this to stop parallel execution, or configure this with the intended number of cores to be used

Alternatively, you can use the Linux taskset command to bind your program with specific CPU cores.

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NEC creates the social values of safety, security, fairness and efficiency to promote a more sustainable world where everyone has the chance to reach their full potential.

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