pandas Roadmap and Beyond

PDEPs: Copy-on-Write, Arrow-backed DataFrames and more

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PyData Prague, April 23rd, 2024

Presentation will be available online:
https://github.com/hkhojasteh

About Hadi

Hadi Abdi Khojasteh

- Background in computer science
- NumFOCUS, PyData community and pandas  core contributor
- Currently working as a Senior Machine Learning Engineer | Innovation Lab and Technical Staff | Technology, Sports Experiences at Deltatre

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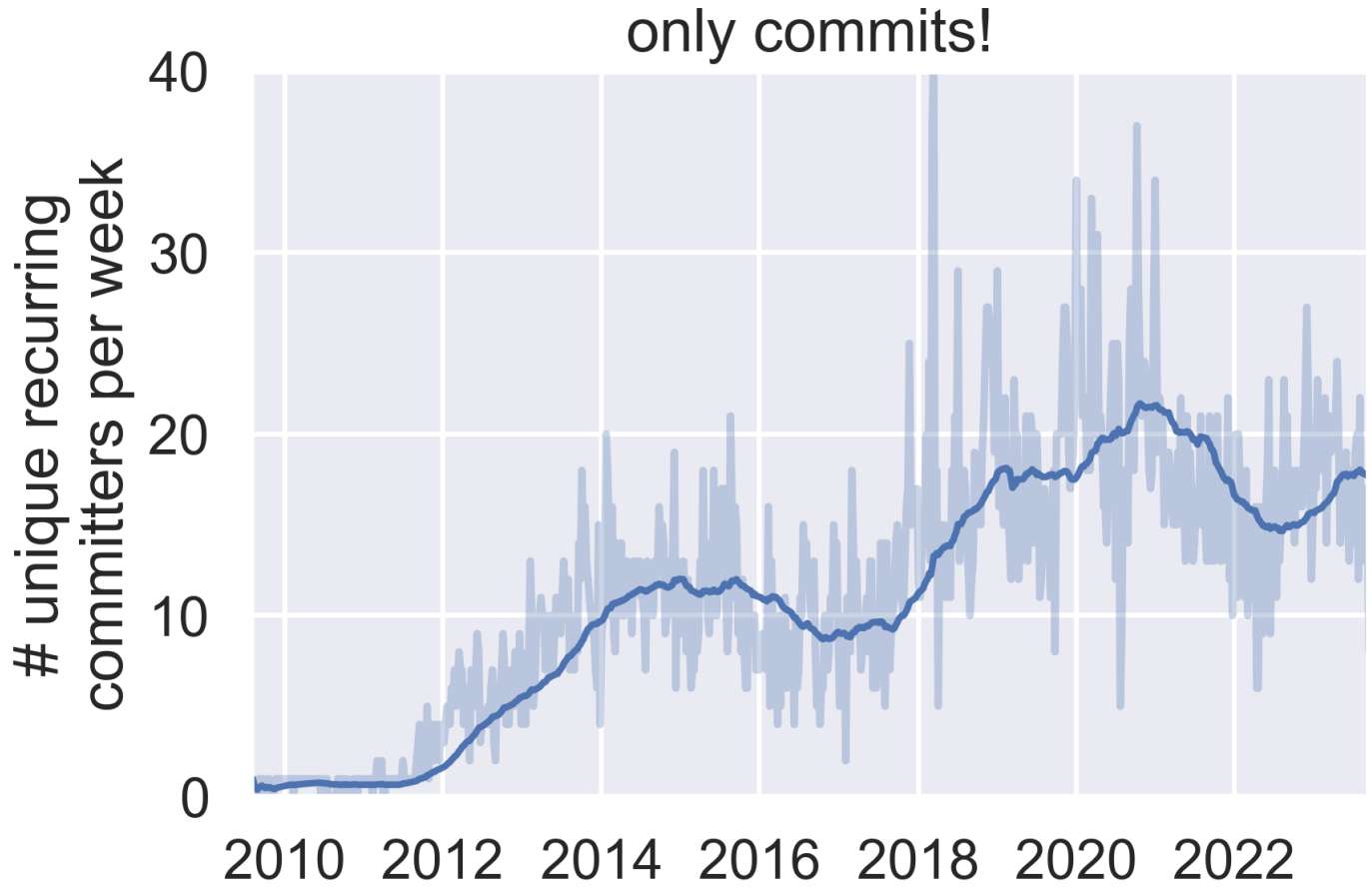
Deltatre Innovation Lab

NUMFOCUS
OPEN CODE = BETTER SCIENCE

pandas contributor community growth



➔ need to update our governance (clarifying roles, updating decision making processes)

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Pandas Enhancement Proposals (PDEPs)

A PDEP is a proposal for a major change in pandas  , similar to a Python PEP or a NumPy NEP.
New process introduced in process in August 2022.

PDEP-1 describes the purpose and guidelines
(currently deciding on voting mechanism for final decisions)
https://pandas.pydata.org/pdeps/0001-purpose-and-guidelines.html

See PDEPs on the pandas roadmap: https://pandas.pydata.org/about/roadmap.html

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Pandas Enhancement Proposals (PDEPs)

See PDEPs on the pandas roadmap: https://pandas.pydata.org/about/roadmap.html

PDEP-4 [Implemented in 2.0]	Consistent datetime parsing
PDEP-6 [Accepted for 3.0]	Ban upcasting in setitem-like operations
PDEP-7 [Open, planned for 3.0]	Consistent copy/view semantics with Copy-on-Write
PDEP-8 [Open, planned for 3.0?]	Inplace methods in pandas
PDEP-10 [Accepted for 3.0]	PyArrow as a required dependency for default string inference
PDEP-11 [Under discussion]	Change the default of dropna to False
PDEP-13 [Under discussion]	Make the Series.apply method operate Series-wise

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Non-nanosecond resolution in Timestamps

pandas only supported Timestamps in nanosecond resolution up until 2.0

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```
>>> pd.Timestamp("1000-01-01")
OutOfBoundsDatetime: Out of bounds nanosecond timestamp: 1000-01-01 00:00:00
```

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pandas 2.0 lifts this restriction!

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>>> pd.Timestamp("1000-01-01")
OutOfBoundsDatetime: Out of bounds nanosecond timestamp: 1000-01-01 00:00:00
```

pandas 2.0 lifts this restriction!

Timestamps can be created in the following units:

- seconds
- milliseconds
- microseconds
- nanoseconds

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How to enable the new resolutions

date_range doesn't yet support non-nano resolutions. But as_unit or astype can be used to convert between units:

```
>>> dr = pd.date_range("2020-01-01", periods=3, freq="D")
>>> dr
DatetimeIndex(['2020-01-01', '2020-01-02'], dtype='datetime64[ns]', freq='D')
```

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How to enable the new resolutions

date_range doesn't yet support non-nano resolutions. But as_unit or astype can be used to convert between units:

```
>>> dr = pd.date_range("2020-01-01", periods=3, freq="D")
>>> dr
DatetimeIndex(['2020-01-01', '2020-01-02'], dtype='datetime64[ns]', freq='D')
```

```
>>> dr.astype("datetime64[s]")
DatetimeIndex(['2020-01-01', '2020-01-02'], dtype='datetime64[s]', freq='D')
```

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How to enable the new resolutions

date_range doesn't yet support non-nano resolutions. But as_unit or astype can be used to convert between units:

The resolution of NumPy arrays is preserved:

```
>>> arr = np.array(['2007-07-13', '2006-01-13'], dtype='datetime64[ms]')
>>> arr
array(['2007-07-13T00:00:00.000', '2006-01-13T00:00:00.000'], dtype='datetime64[ms]')

>>> pd.Series(arr)
0 2007-07-13
1 2006-01-13
dtype: datetime64[ms]
```

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PDEP-4: Consistent datetime parsing

Old behaviour: when not specifying a specific format, each value was being parsed independently:

```
>>> pd.to_datetime(['12-01-2000 00:00:00', '13-01-2000 00:00:00'])
DatetimeIndex(['2000-12-01', '2000-01-13'], dtype='datetime64[ns]', freq=None)
```

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PDEP-4: Consistent datetime parsing

Old behaviour: when not specifying a specific format, each value was being parsed independently:

```
>>> pd.to_datetime(['12-01-2000 00:00:00', '13-01-2000 00:00:00'])
DatetimeIndex(['2000-12-01', '2000-01-13'], dtype='datetime64[ns]', freq=None)
```

New behaviour in pandas 2.0: if no format is specified, the format will be guessed from the first string and applied to all values

```
>>> pd.to_datetime(['12-01-2000 00:00:00', '13-01-2000 00:00:00'])
...
# ValueError: time data "13-01-2000 00:00:00" doesn't match format "%m-%d-%Y %H:%M:%S".
# You might want to try:
# - passing `format` if your strings have a consistent format;
# - passing `format='ISO8601'` if your strings are all ISO8601 but not necessarily in exactly the sam
# - passing `format='mixed'`, and the format will be inferred for each element individually. You migh
```

Full details:
https://pandas.pydata.org/pdeps/0004-consistent-to-datetime-parsing.html

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PDEP-7: Consistent copy/view semantics in Pandas with Copy-on-Write

a.k.a. Getting rid of the SettingWithCopyWarning

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Current situation: SettingWithCopyWarning

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
>>> subset = df[df["A"] > 1]
>>> subset.loc[1, "C"] = 10

# SettingWithCopyWarning:
# A value is trying to be set on a copy of a slice from a DataFrame.
# Try using .loc[row_indexer,col_indexer] = value instead
#
# See the caveats in the documentation: ...
```

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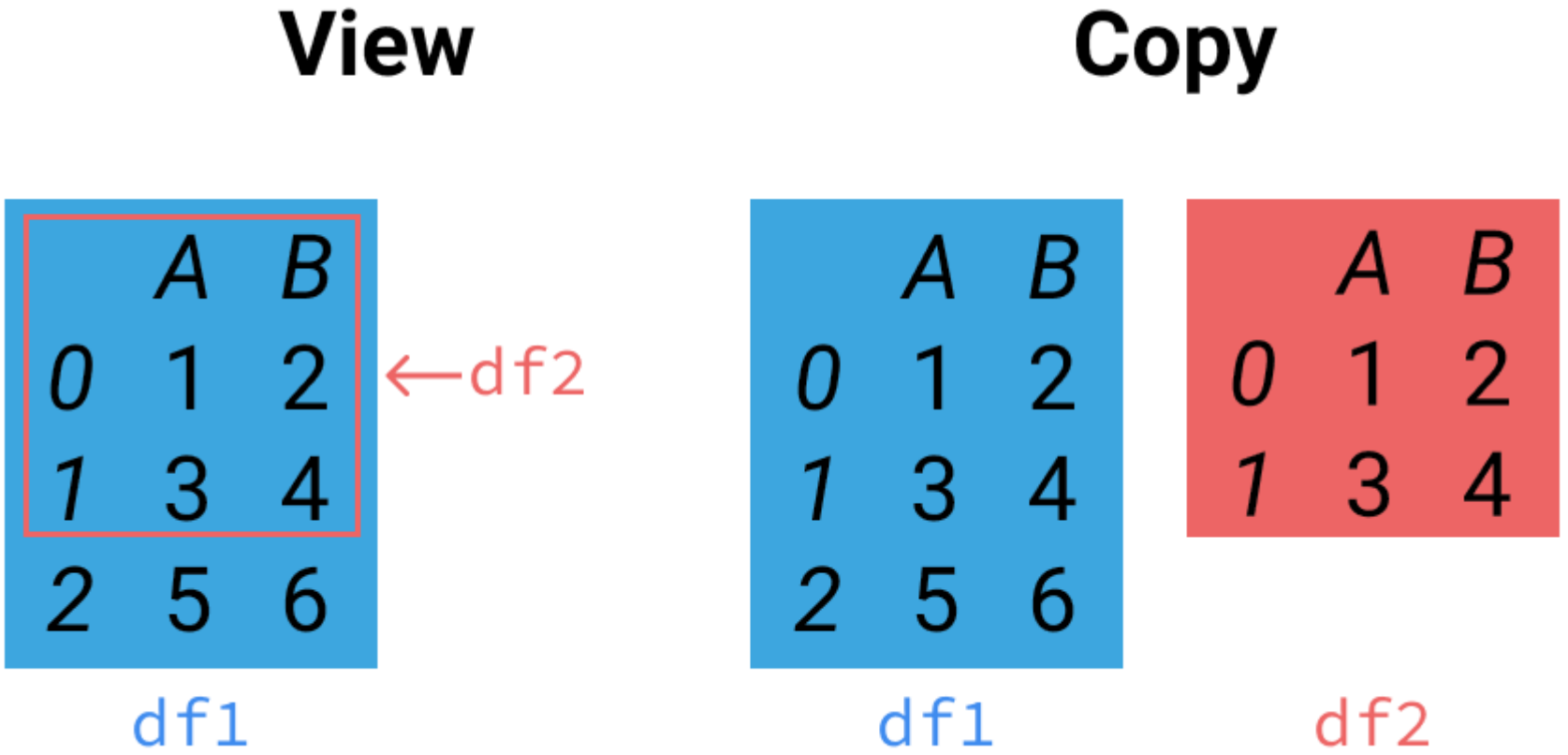
Current situation: copy vs view



Images from https://www.dataquest.io/blog/settingwithcopywarning/

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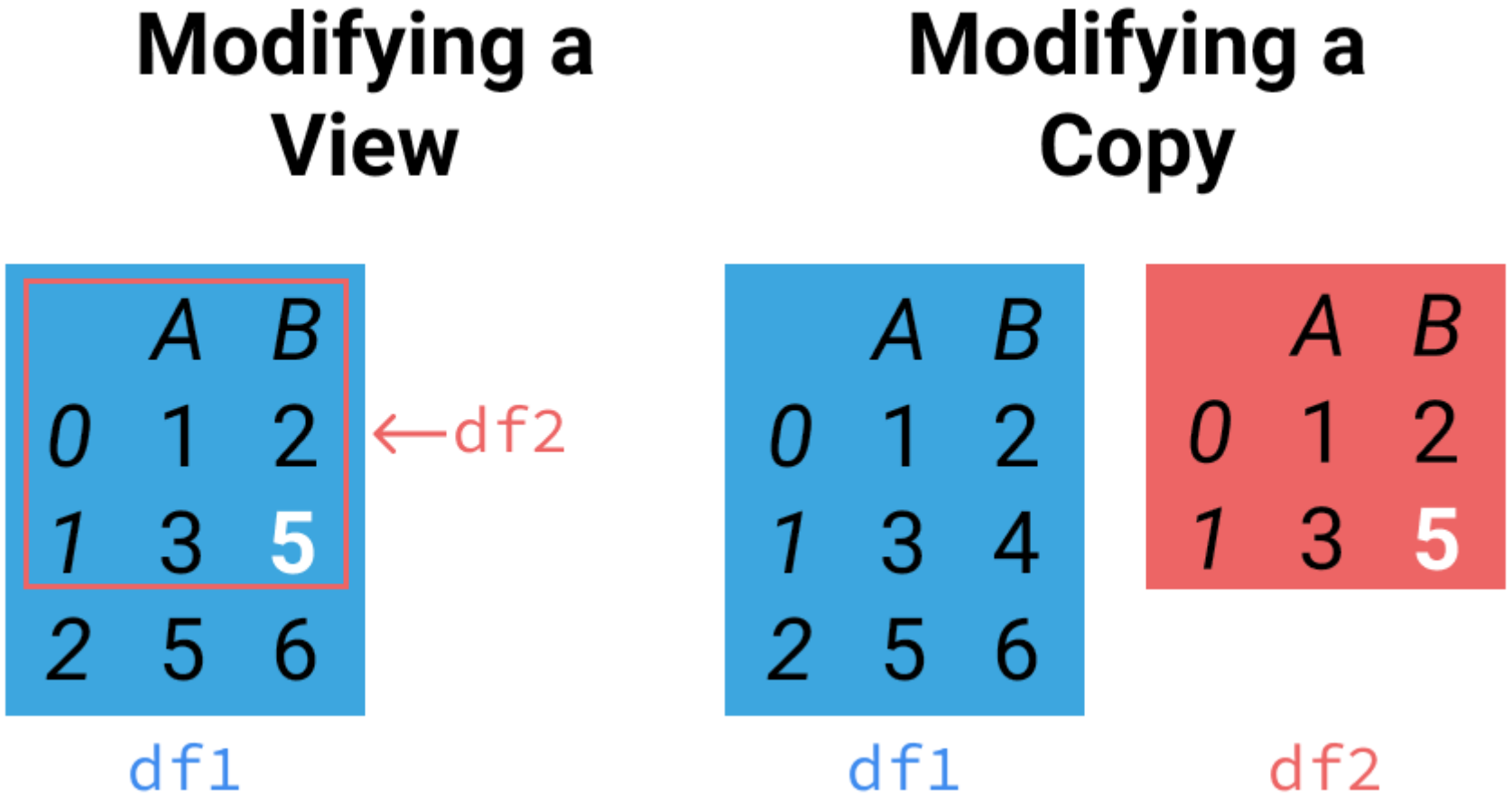
Current situation: copy vs view



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The SettingWithCopyWarning

How to "solve" the warning?

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How to "solve" the warning?

I want do update df -> setitem in one go

```
>>> df[df["A"] > 1]["C"] = 10        # this doesn't work
>>> df["C"][df["A"] > 1] = 10        # this works
>>> df.loc[df["A"] > 1, "C"] = 10    # this works
```

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The SettingWithCopyWarning

How to "solve" the warning?

I want do update df -> setitem in one go

```
>>> df[df["A"] > 1]["C"] = 10        # this doesn't work
>>> df["C"][df["A"] > 1] = 10        # this works
>>> df.loc[df["A"] > 1, "C"] = 10    # this works
```

I don't want to update df -> explicit (unnecessary) copy()

```
>>> subset = df[df["A"] > 1].copy()
>>> subset["C"] = 10
```

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Current situation

Problems with the current copy / view semantics of pandas:

- This is confusing for many users
- You need to be aware of copy/view details of NumPy
- You need defensive (and unnecessary) copying to avoid the warning

Can we do better?

A proposal for simplified behaviour using a single rule:

- Any DataFrame or Series derived from another in any way (e.g. with an indexing operation) always behaves as a copy

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Or put differently, the implication is:

- Mutating a DataFrame or Series only changes the object itself, and not any other.
  If you want to change values in a DataFrame or Series, you can only do that by directly mutating the DataFrame/Series at hand.

Can we do better?

A proposal for simplified behaviour using a single rule:

- ❑ Any DataFrame or Series derived from another in any way (e.g. with an indexing operation) always behaves as a copy

Advantages:

- **A simpler, more consistent user experience**
- We can get rid of the SettingWithCopyWarning (since there is no confusion about whether we are mutating a view or a copy)
- We would no longer need defensive copying in many places in pandas, improving memory usage and performance

Previous example modifying a subset

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
>>> subset = df[df["A"] > 1]
>>> subset.loc[1, "C"] = 10
```

Did df change as well?

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Previous example modifying a subset

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
>>> subset = df[df["A"] > 1]
>>> subset.loc[1, "C"] = 10
```

Did df change as well?

No, subset is a different object, so mutating subset does not change df.

And the answer is the same regardless how subset was created (selecting rows or columns, with a slice, mask, or list indexer, ..)

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The SettingWithCopyWarning

With current pandas (trying to update df):

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
# two examples of chained assignment
>>> df["C"][df["A"] > 1] = 10   # this works
>>> df[df["A"] > 1]["C"] = 10   # this doesn't work
```

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The SettingWithCopyWarning

With current pandas (trying to update df):

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
# two examples of chained assignment
>>> df["C"][df["A"] > 1] = 10   # this works
>>> df[df["A"] > 1]["C"] = 10   # this doesn't work
```

With new behaviour: both examples don't work

```
>>> df["C"][df["A"] > 1] = 10   # this doesn't work
>>> df[df["A"] > 1]["C"] = 10   # this doesn't work
```

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The SettingWithCopyWarning

With current pandas (trying to update df):

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
# two examples of chained assignment
>>> df["C"][df["A"] > 1] = 10   # this works
>>> df[df["A"] > 1]["C"] = 10   # this doesn't work
```

With new behaviour: chained assignment will never work -> we don't need the general warning.

But to help the transition, we can specifically warn about chained assignment not working:

```
>>> df["C"][df["A"] > 1] = 10

# ChainedAssignmentError: A value is trying to be set on a copy of a DataFrame
# or Series through chained assignment.
# When using the Copy-on-Write mode, such chained assignment never works ...
```

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Can we do better?

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- ❑ Any DataFrame or Series derived from another in any way (e.g. with an indexing operation) always behaves as a copy

Advantages:

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- **We would no longer need defensive copying in many places in pandas, improving memory usage and performance**

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The SettingWithCopyWarning

With current pandas (not wanting to update df):

```
>>> df = pd.DataFrame({"A": [1, 2], "B": [3, 4], "C": [5, 6]})
>>> subset = df[df["A"] > 1].copy()
...
>>> subset["C"] = 10
```

With new behaviour: additional copy() is no longer needed to avoid the warning.

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Avoiding copies with Copy-on-Write

The usage of view vs copy can become an internal implementation detail

➔ We can avoid copies by default using Copy-on-Write!

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Small benchmark:

create DataFrame of 2 million rows by 30 columns (mix of float, integer and string columns)

```
import pandas as pd
import numpy as np

N = 2_000_000
int_df = pd.DataFrame(np.random.randint(1, 100, (N, 10)), columns=[f"col_{i}" for i in range(10)])
float_df = pd.DataFrame(np.random.random((N, 10)), columns=[f"col_{i}" for i in range(10, 20)])
str_df = pd.DataFrame("a", index=range(N), columns=[f"col_{i}" for i in range(20, 30)])

df = pd.concat([int_df, float_df, str_df], axis=1)
```

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Small benchmark:

create DataFrame of 2 million rows by 30 columns (mix of float, integer and string columns)

```
%%timeit
(df.rename(columns={"col_1": "new_index"})
   .assign(sum_val=df["col_1"] + df["col_2"])
   .drop(columns=["col_10", "col_20"])
   .astype({"col_5": "int32"})
   .reset_index()
   .set_index("new_index")
)
2.45 s ± 293 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

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   .astype({"col_5": "int32"})
   .reset_index()
   .set_index("new_index")
)
2.45 s ± 293 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
# with Copy-on-Write enabled
13.7 ms ± 286 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```
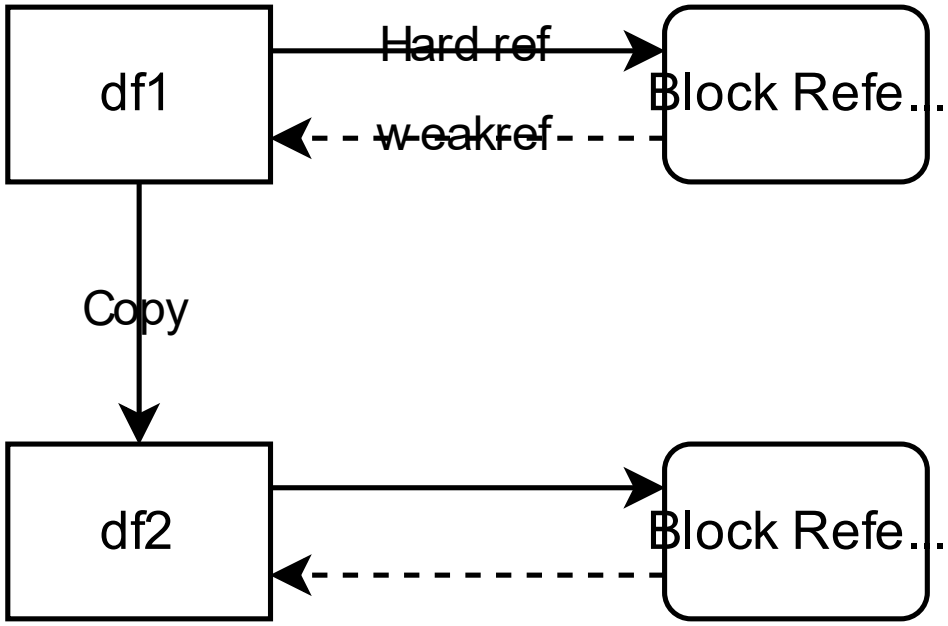

Hiding copy/view details with Copy-on-Write

When an operations makes an actual copy of the data

➔ each DataFrame references its own data

```
df2 = df1.copy()
```



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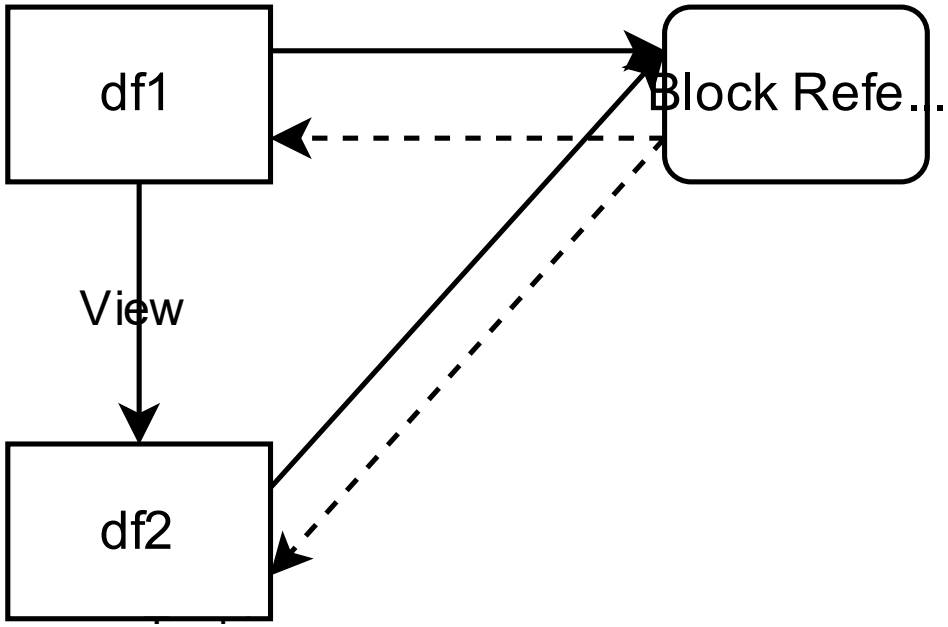
Hiding copy/view details with Copy-on-Write

When an operations can use a view for the result

➔ both reference the same data

```
df2 = df1.reset_index()
```



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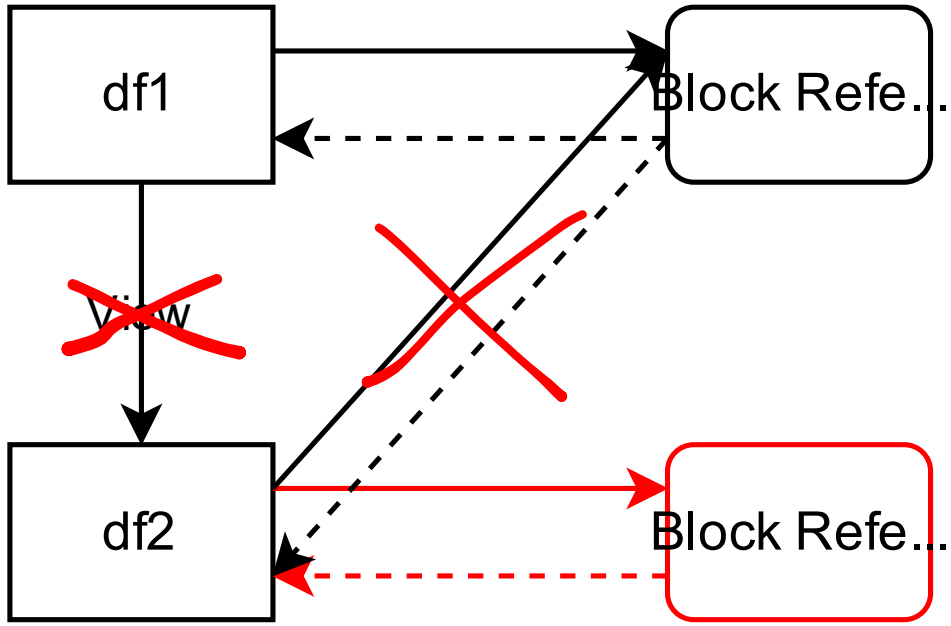
Hiding copy/view details with Copy-on-Write

Modifying a view or its parent (df1 or df2) will trigger a copy (a "copy on write")

➔ each DataFrame again owns its own memory.

```
df2 = df1.reset_index()
df2.loc[1, "C"] = 10
```



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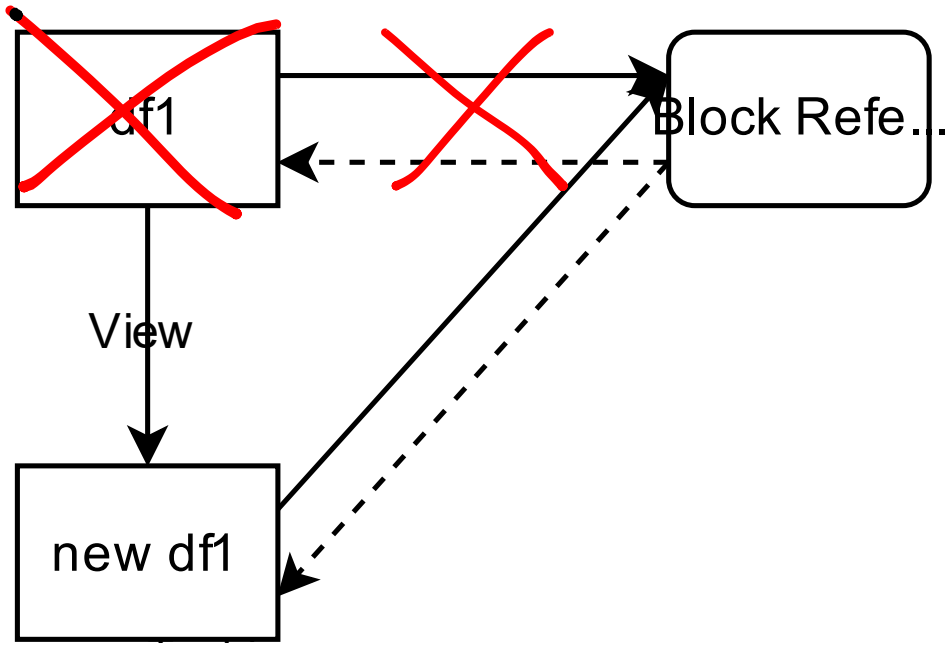
Hiding copy/view details with Copy-on-Write

Do you want to avoid this copy when modifying df2, and no longer need df1? You can for example reassign to the same variable such that the original df1 goes out of scope.

```
df1 = df1.reset_index()
```



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How do I try this?

Enable it in pandas 2.0 :

```
import pandas as pd
pd.options.mode.copy_on_write = True
```

- We encourage you to try it out!
- We expect it to become the default behaviour in pandas 3.0
- Blogposts:
  - https://jorisvandenbossche.github.io/blog/2022/04/07/pandas-copy-views/
  - https://medium.com/towards-data-science/a-solution-for-inconsistencies-in-indexing-operations-in-pandas-b76e10719744
- Full proposal: https://github.com/pandas-dev/pandas/pull/51463/

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PDEP-10: PyArrow as a required dependency for default string inference implementation

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Arrow-backed data types

Using PyArrow arrays to store the data of a DataFrame.

Apache Arrow *defines a language-independent columnar memory format for flat and hierarchical data, organized for efficient analytic operations on modern hardware like CPUs and GPUs.*

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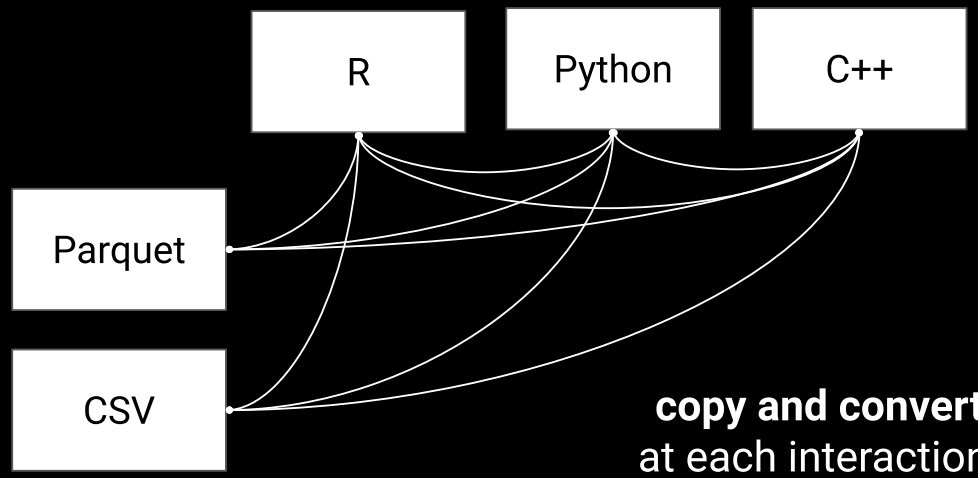
Apache Arrow is a specification defining a common, language-agnostic in-memory representation for columnar data

\+ A multi-language toolbox for accelerated data interchange and in-memory processing

Arrow Data Interchange



copy and convert happens at each interaction, incurring serialization costs

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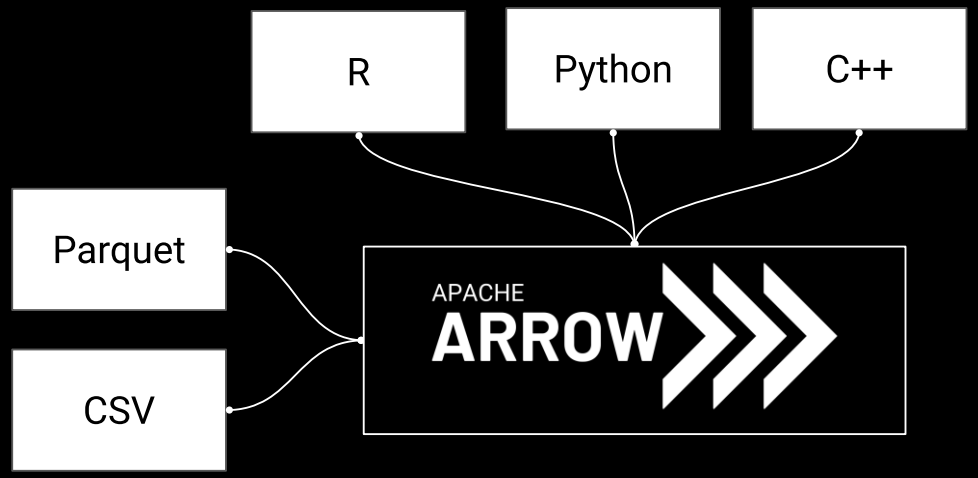
Apache Arrow is a specification defining a common, language-agnostic in-memory representation for columnar data

\+ A multi-language toolbox for accelerated data interchange and in-memory processing

Arrow Data Interchange



Arrow provides a standard in-memory format and reduces serialization costs when connecting systems

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Avoid object dtype for strings by default

Currently:

```
>>> pd.Series(["a", "b", "c"])
0 a
1 b
2 c
dtype: object
```

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Avoid object dtype for strings by default

Currently:

```
>>> pd.Series(["a", "b", "c"])
0 a
1 b
2 c
dtype: object
```

Future behaviour:

```
>>> pd.options.future.infer_string = True
>>> pd.Series(["a", "b", "c"])
0 a
1 b
2 c
dtype: string[pyarrow]
```

Planned for 3.0 by default, but you can already opt-in starting with pandas 2.1

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PyArrow-backed string dtype

PyArrow offers fast and efficient in-memory string operations.

This provides:

- significantly improved performance compared to NumPy's object dtype with Python str operations
- smaller memory footprint

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PyArrow-backed string dtype

PyArrow offers fast and efficient in-memory string operations.

This provides:

- significantly improved performance compared to NumPy's object dtype with Python str operations
- smaller memory footprint
- compatible with existing object-dtype-based string methods (all .str. string accessor methods keep working)

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Let's look at some performance/memory comparisons

```
import string
import random

import pandas as pd

def random_string() -> str:
    return "".join(random.choices(string.printable, k=random.randint(10, 100)))

ser_object = pd.Series([random_string() for _ in range(1_000_000)])
ser_string = ser_object.astype("string[pyarrow]")
```

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Let's look at some performance/memory comparisons

str.length

```
In[1]: %timeit ser_object.str.len()
118 ms ± 260 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)

In[2]: %timeit ser_string.str.len()
24.2 ms ± 187 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

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Let's look at some performance/memory comparisons

str.length

```
In[1]: %timeit ser_object.str.len()
118 ms ± 260 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)

In[2]: %timeit ser_string.str.len()
24.2 ms ± 187 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

str.startswith

```
In[3]: %timeit ser_object.str.startswith("a")
136 ms ± 300 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)

In[4]: %timeit ser_string.str.startswith("a")
11 ms ± 19.8 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

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Let's look at some performance/memory comparisons

memory footprint

```
In [5]: "{:.2f} MiB".format(ser_object.memory_usage(deep=True) / 1024**2)
Out[5]: '106.82 MiB'

In [6]: "{:.2f} MiB".format(ser_string.memory_usage(deep=True) / 1024**2)
Out[6]: '56.28 MiB'
```

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PyArrow-backed string dtype by default in 3.0

- PyArrow will become a **required** dependency of pandas starting with pandas 3.0
- The PyArrow-backed string dtype will be used by default (no more object dtype for strings!)

How do I try this now?

Enable it in pandas 2.1:

```
pd.options.future.infer_string = True
```

- PDEP: https://pandas.pydata.org/pdeps/0010-required-pyarrow-dependency.html
- Blogpost of Patrick Höfler about improvements in pandas and dask: https://towardsdatascience.com/utilizing-pyarrow-to-improve-pandas-and-dask-workflows-2891d3d96d2b

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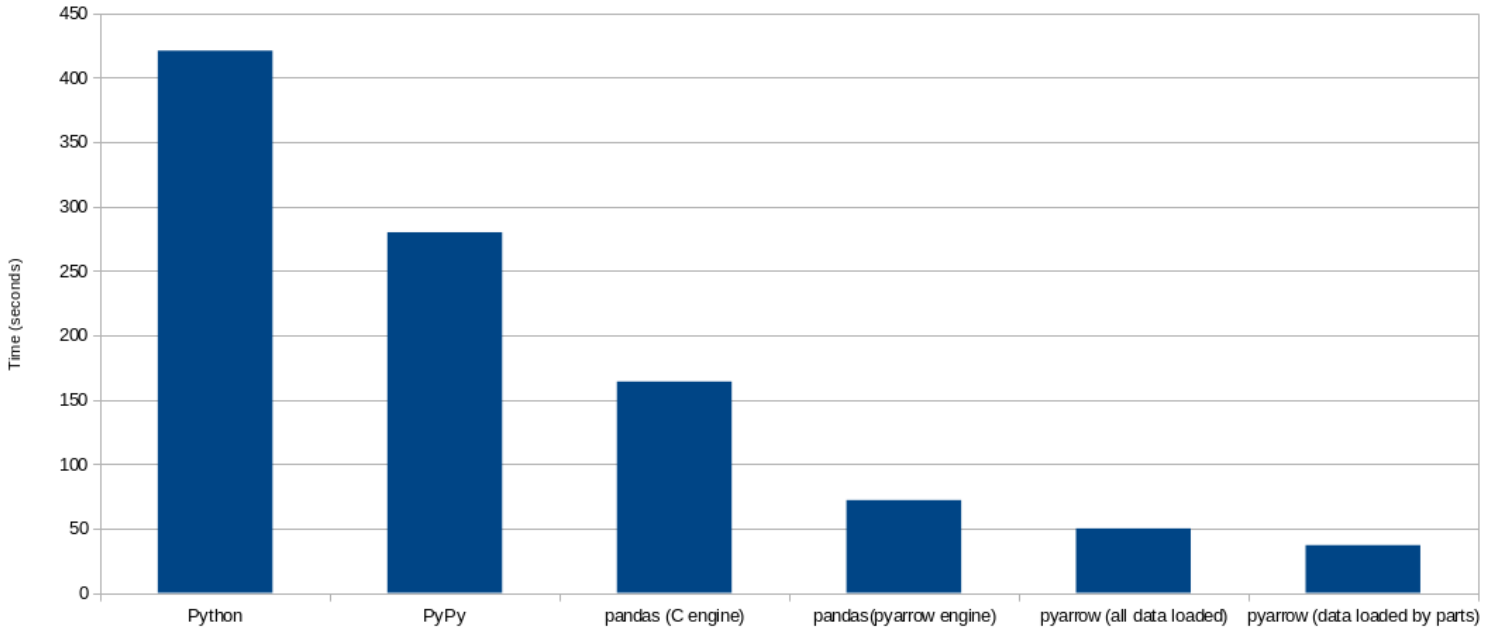
Speeding up I/O operations with PyArrow engine

Some I/O functions gained an engine keyword to parse the input with PyArrow.

- read_csv and read_json can dispatch to PyArrow readers.
- read_parquet and read_orc use PyArrow natively to read the input.

➔ Huge performance improvements and uses multithreading with Zero-copy



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PyArrow offers support for a wide variety of dtypes (not well supported by pandas right now):

- string, bytes, decimal, date, explicit null-datatype, nested data and many more.

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Experimental ArrowDtype for using any Arrow type in a column

pd.ArrowDtype or f"{dtype}[pyarrow]" creates Arrow-backed columns

```
>>> import pyarrow as pa
>>> pd.Series([1, 2, 3], dtype=pd.ArrowDtype(pa.int64()))
0 1
1 2
2 3
dtype: int64[pyarrow]

>>> pd.Series([1, 2, 3], dtype="int64[pyarrow]")
```

These columns use the PyArrow memory layout and compute functionality.

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Experimental ArrowDtype for using any Arrow type in a column

```
>>> import pyarrow as pa
>>> pd.Series([1, 2, 3], dtype=pd.ArrowDtype(pa.int64()))
0 1
1 2
2 3
dtype: int64[pyarrow]
```

These columns use the PyArrow memory layout and compute functionality.

➔ opt-in using new dtype_backend="pyarrow" keyword in IO methods, or df.convert_dtypes(dtype_backend="pyarrow") to convert afterwards

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Dispatching to pyarrow.compute

The ExtensionArray interface of pandas dispatches to compute functions of PyArrow.

```
In [3]: ser = pd.Series(np.random.randint(1, 100, (5_000_000, )))
```

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In [3]: ser = pd.Series(np.random.randint(1, 100, (5_000_000, )))
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```
In [4]: %timeit ser.unique()
10.6 ms ± 31.8 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
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```
n [5]: ser_arrow = ser.astype(pd.ArrowDtype(pa.int64()))
In [6]: %timeit ser_arrow.unique()
6.71 ms ± 6.8 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

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Dispatching to pyarrow.compute

The ExtensionArray interface of pandas dispatches to compute functions of PyArrow.

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6.71 ms ± 6.8 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

➔ PyArrow can provide a significant performance improvement

Not every method of pandas supports the compute functionality of PyArrow yet.

PDEP-6: Ban upcasting in setitem-like operations

```
df = pd.DataFrame({"a": [1, 2, 3]})
df.loc[1, "a"] = 3.5
df.loc[1, "a"] = "3"
```

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PDEP-6: Ban upcasting in setitem-like operations

```
df = pd.DataFrame({"a": [1, 2, 3]})
df.loc[1, "a"] = 3.5
df.loc[1, "a"] = "3"
```

When assigning a value into a Series that would cause the dtype to change, it is not clear what the user wants to happen. Different users may want different things.

➔ pandas shoudn't guess!

Summary: Assignments into an existing Series that would change the dtype will now raise.

Full proposal: https://github.com/pandas-dev/pandas/pull/50402

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PDEP-8: In-place methods in pandas

Proposal (still being discussed!):

- The inplace parameter will be deprecated and removed from any method that can never be done inplace
- The inplace parameter is kept only in a few methods such as fillna()

For example, replace

```
df.reset_index(inplace=True)
```

with

```
df = df.reset_index()
```

Full proposal: https://github.com/pandas-dev/pandas/pull/51466

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PDEP-11: Change the default of dropna to False

Motivating Example: Compute the average time for groups of 3 runners.

```
df = pd.read_excel("runner_times.xlsx")
df.value_counts("group")
result = df.groupby("group")[["seconds"]].mean()
result.to_excel("group_means.xlsx")
```

- Some methods (stack, pivot_table) do not behave well with dropna=False
  - You can try the new implementation of stack in version 2.1!
- What should we do with mode?
  - If mode is counting values, then it should have dropna=False.
  - If mode is a stats method like mean and median, then it should have skipna=True

Full proposal: https://github.com/pandas-dev/pandas/pull/53094

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pandas 2.2.0 released on January 19th!

Upcoming changes in pandas 3.0 which bring two bigger changes to the default behavior of pandas:

- Copy-on-Write
- Dedicated string data type (backed by Arrow) by default

New enhancements on

- pandas Apache Arrow ADBC Driver support in to_sql and read_sql; significant performance improvements
- Create a Series based on one or more conditions; Series.case_when()
- Series.struct and Series.list accessor for PyArrow structured data

And many more! See full release notes at https://pandas.pydata.org/docs/dev/whatsnew/v2.2.0.html

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Thanks to all contributors!

Pandas  is a community project,
and everything we talked about is the result of this community of contributors

A total of 162 people contributed to the 2.2.0 (January 19, 2024) release!

(and that's only counting commits on the main repo)

You can become part of this community as well!

https://pandas.pydata.org/docs/development/contributing.html

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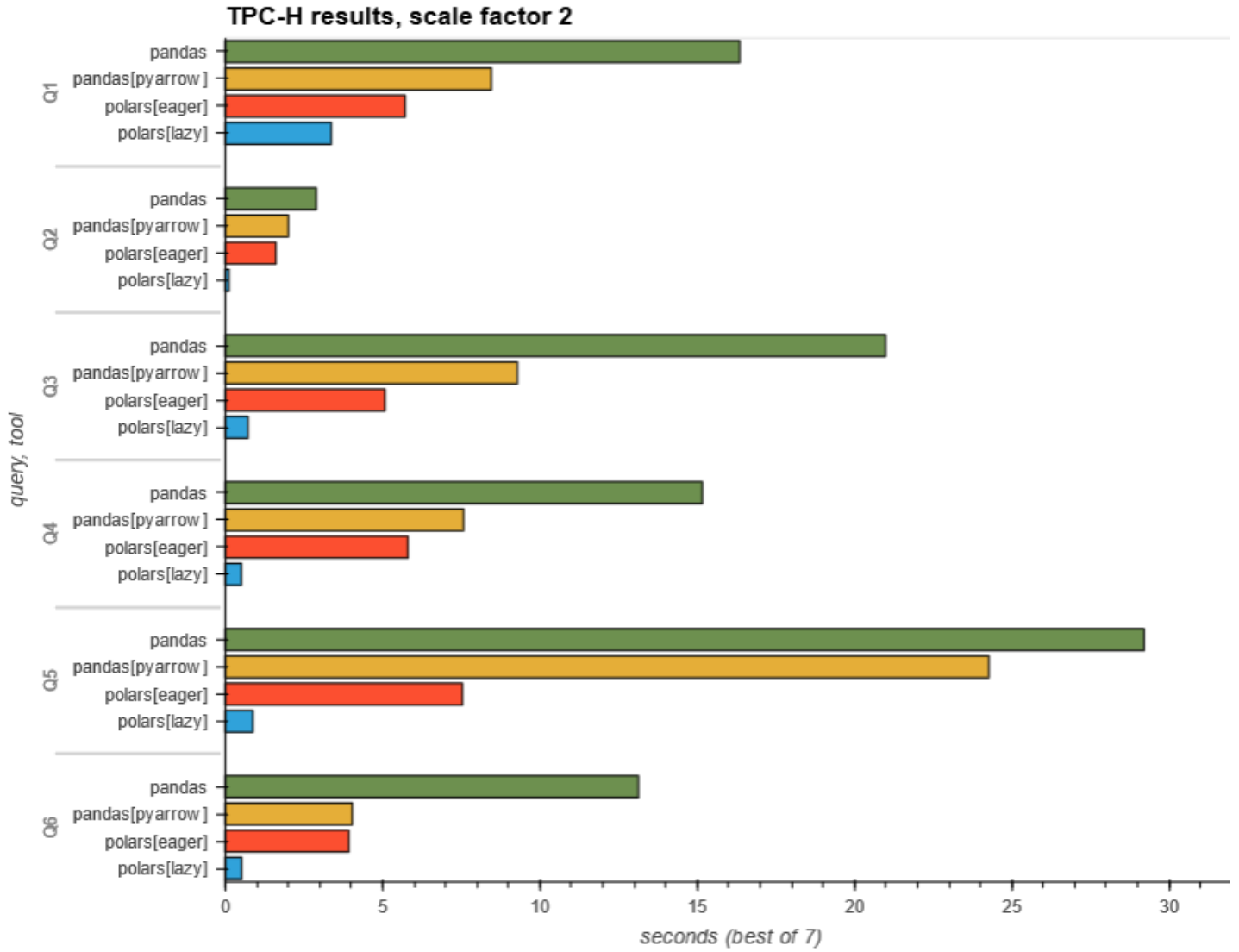
pandas vs Polars / query optimization and multi threading



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pandas + Polars / Interoperability example

```
loaded_pandas_data = pandas.read_sas(fname)

polars_data = polars.from_pandas(loaded_pandas_data)
# perform operations with pandas polars

to_export_pandas_data = polars.to_pandas(use_pyarrow_extension_array=True)
to_export_pandas_data.to_latex()
```

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Pay attention to warnings!

571

Found this on github...

```
import warnings
warnings.simplefilter(action='ignore', category=FutureWarning)

import pandas
```

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edited Feb 20, 2020 at 8:37
smci
smci's 33.4k • 21 • 116 • 148

answered Apr 3, 2013 at 3:19
bdiamante
16.8k • 6 • 41 • 47

61 nb: put the `warnings....ignore` *before* the `import pandas...` to cause the `FutureWarning` to be ignored. – michael Dec 8, 2017 at 13:31

29 Hey I'm getting the future warning despite adding these lines. – Eswar Oct 6, 2020 at 17:19

It's working. Vote up. – Zbyszek Feb 14 at 14:16

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Thank you for your attention :)

pandas Roadmap and Beyond
PDEPs: Copy-on-Write, Arrow-backed DataFrames and more

Find me in

Presentation will be available online:
https://github.com/hkhojasteh

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