Processing large-scale data efficiently: An introduction to the R package 'data.table'.

Research Data Scotland

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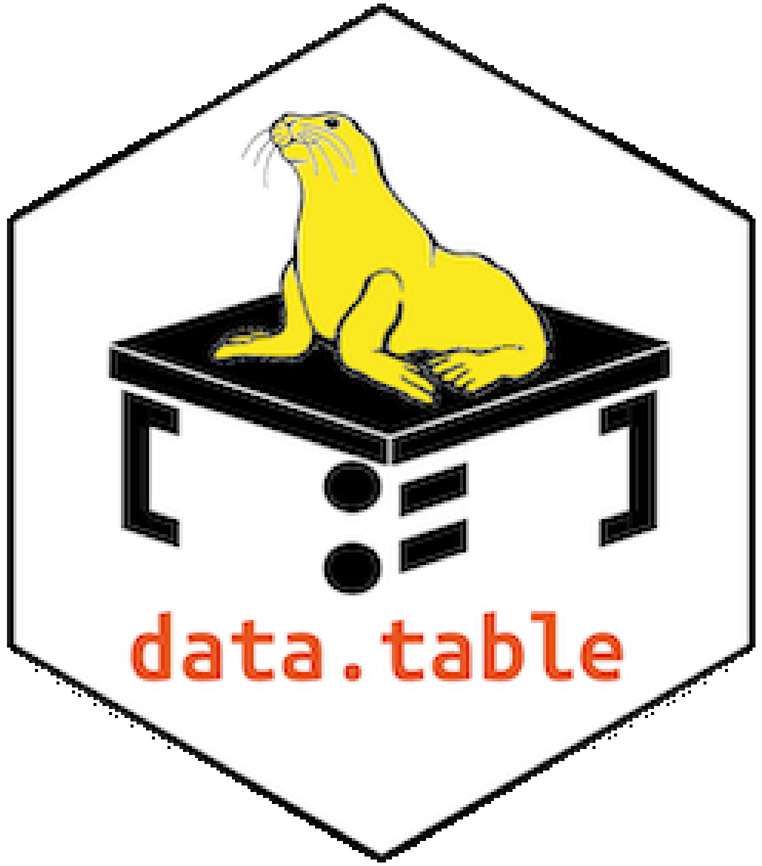
Outline

Introducing 'data.table'

Hands-on Session

Q&A



Source: https://rdatatable.gitlab.io/data.table/

Introducing ‘data.table’

What will be faster: A Ferrari or a Honda?

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What will be faster: A Ferrari or a Honda?

Photo by Stefano Probst on Unsplash

vs.

Photo by Brad armore on Unsplash

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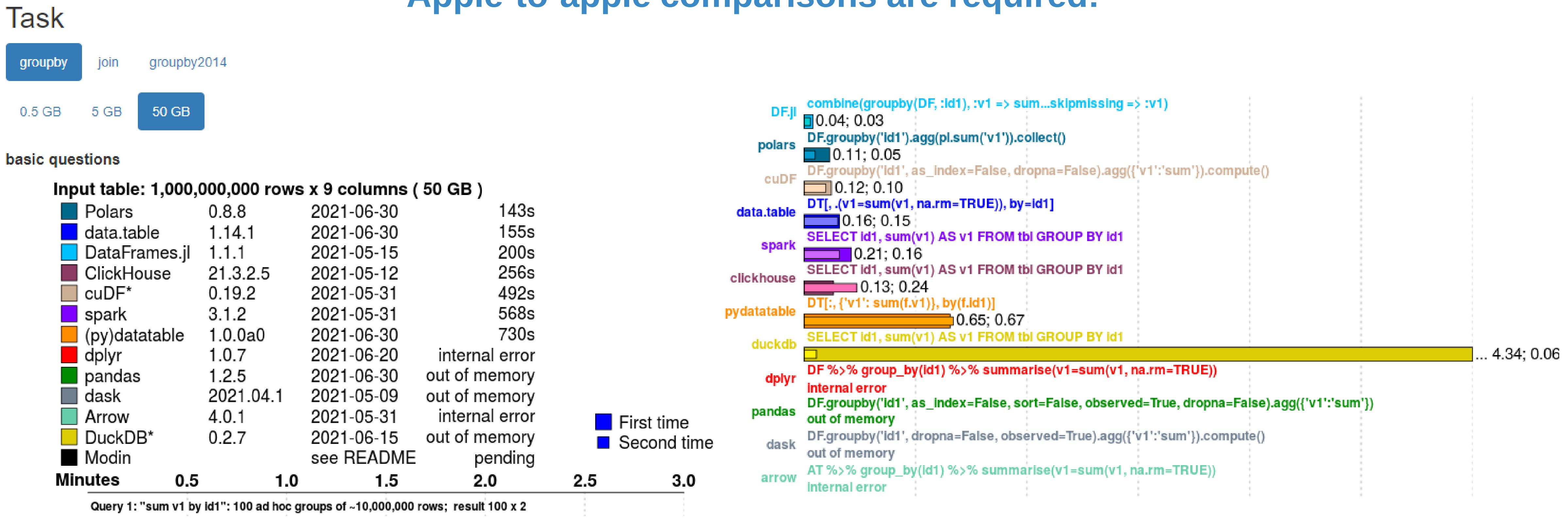
Apple-to-apple comparisons are required!



Task

groupby | join | groupby2014

0.5 GB | 5 GB | 50 GB

basic questions

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

🟦	Polars	0.8.8	2021-06-30	143s
🟦	data.table	1.14.1	2021-06-30	155s
🟦	DataFrames.jl	1.1.1	2021-05-15	200s
🟪	ClickHouse	21.3.2.5	2021-05-12	256s
🟫	cuDF*	0.19.2	2021-05-31	492s
🟪	spark	3.1.2	2021-05-31	568s
🟧	(py)datatable	1.0.0a0	2021-06-30	730s
🟥	dplyr	1.0.7	2021-06-20	internal error
🟩	pandas	1.2.5	2021-06-30	out of memory
⬜	dask	2021.04.1	2021-05-09	out of memory
🟩	Arrow	4.0.1	2021-05-31	internal error
🟨	DuckDB*	0.2.7	2021-06-15	out of memory
⬛	Modin		see README	pending

🟦 First time
🟦 Second time

```
DF.jl        combine(groupby(DF, :id1), :v1 => sum∘skipmissing => :v1)
             0.04; 0.03
polars       DF.groupby('id1').agg(pl.sum('v1')).collect()
             0.11; 0.05
cuDF         DF.groupby('id1', as_index=False, dropna=False).agg({'v1':'sum'}).compute()
             0.12; 0.10
data.table   DT[, .(v1=sum(v1, na.rm=TRUE)), by=id1]
             0.16; 0.15
spark        SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1
             0.21; 0.16
clickhouse   SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1
             0.13; 0.24
pydatatable  DT[:, {'v1': sum(f.v1)}, by(f.id1)]
             0.65; 0.67
duckdb       SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1
             ... 4.34; 0.06
dplyr        DF %>% group_by(id1) %>% summarise(v1=sum(v1, na.rm=TRUE))
             internal error
pandas       DF.groupby('id1', as_index=False, sort=False, observed=True, dropna=False).agg({'v1':'sum'})
             out of memory
dask         DF.groupby('id1', dropna=False, observed=True).agg({'v1':'sum'}).compute()
             out of memory
arrow        AT %>% group_by(id1) %>% summarise(v1=sum(v1, na.rm=TRUE))
             internal error
```

Query 1: "sum v1 by id1": 100 ad hoc groups of ~10,000,000 rows; result 100 x 2

Source: https://h2oai.github.io/db-benchmark/

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Scene Setting

1) Routinely collected data has always been large - and will only get larger (e.g. high-dimensional smart data, real-time data, omics data, CTGAN synthetic data)

2) Memory (RAM) and processing capacity (CPU) have remained limited resources

While R is a fantastic programming language, “standard” R (e.g. through base or tidyverse) is not an efficient/safe/futureproof/portable/updateable/….. way of working

Even worse! The limitations of “standard” R will fuel the problems that come from 1) and 2)

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“Standard” R’s limitations

1) By default, R uses 1 core – but many more are available on most machines (→ CPU + time)

2) By default, R has a “copy-on-modify behaviour” (→ RAM + time)

3) Dependencies, portability, backward compatibility: Updates vs. old code (→ lots of time ….)

4) R Code can get long, especially when using long chains of pipes (→ even more time …)

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“Standard” R’s limitations vs. data.table

1) By default, R uses 1 core – but many more are available on most machines (→ CPU + time)
data.table parallelises whenever this is easily done, running compiled C/C++ underneath

2) By default, R has a “copy-on-modify behaviour” (→ RAM + time)
data.table modifies on reference (“ := “) and uses pointers, requiring less working RAM

3) Dependencies, portability, backward compatibility: Updates vs. old code (→ lots of time ….)
data.table has no dependencies other than R >= Version 3.1 (10+ years old)

4) R Code can get long, especially when using long chains of pipes (→ even more time …)
data.table has short and expressive code, similar to high-level programming languages

Introducing ‘data.table’

What is data.table?

1) A selection of functions, optimised to work efficiently with large amounts of data (e.g., fread, fwrite, or for reshaping long-wide / wide-long)

2) A separate dialect for R, with some degree of similarity to SQL or C/C++ code

3) A unique chance to learn about R and computing, with the aim of improving processes and futureproofing our work

Source: https://rdatatable.gitlab.io/data.table/

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Standard ‘data.table’ notation

Standard format 1: data[i , j] → basic format when not operating on groups

Standard format 2: data[i , j , by] → when operating by group

“data”	is our dataset
“i”	subset of “data” based on row information (“subset on observations/rows”)
“j”	states what to execute for the columns (“execute on variables/columns”)
“by”	defines whether “i” and “j” should be done by groups

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How to read data.table?

data[sex == “Male”,]   → subset where sex is “Male”, nothing to execute

data[, V2 := V1+1]   → nothing to subset, create a new variable “V2” which is “V1+1”

data[sex == “Male”, V2 := V1+1]   → subset where sex is “Male”, then create V2…

data[sex == “Male”, .(V2 = max(V1))] → subset where sex is “Male”, then return a new variable

data[, .(V2 = max(V1)), by = c(“sex”)]   → no subset, return new variable by group (“sex” variable)

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Any guesses?

Situation: A three-variable dataset (ID, age, income) reflecting yearly income data (repeated obs.)
data2 <- data[age >= 16, .(income_median = median(income)), by = c(“ID”)]

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Any guesses?

Situation: A three-variable dataset (ID, age, income) reflecting yearly income data (repeated obs.)

```
data2 <- data[age >= 16, .(income_median = median(income)), by = c(“ID”)]
```

… assign to a new object data2 something that comes out of data, new data will have 1 row per ID
… subset is what comes before the comma: select those aged 16 or older
… the new variable “income_median” is the median income of all recorded incomes of the subset
… which was established separately for all “IDs” (e.g., there are multiple income records per “ID”)

Hands-on Session

All course materials are available on GitHub!

No account required, a .zip bundle can be downloaded

Repository: 2024_RDS_DT

https://github.com/AndreasxHoehn/2024_RDS_DT

Hands-on Session

Objectives: Big Picture + Transferable Skills + Strong Foundation

1) Benchmarking time: ‘microbenchmark::microbenchmark()’

2) Benchmarking memory: ‘object.size()’ and variable types

3) Tracing the location of objects within ‘tracemem()’

4) Introduction to ‘data.table’ - basic functions, subsets, creating new variables, group by operations, reshaping data “wide to long” & “long to wide”

Further Resources

data.table on cran: https://cran.r-project.org/web/packages/data.table/

Benchmarking data.table operations: https://tysonbarrett.com//jekyll/update/2019/10/06/datatable_memory/

Benchmarking joins: https://tysonbarrett.com/jekyll/update/2019/10/11/speed_of_joins/

A good basic data.table intro: https://atrebas.github.io/post/2020-06-17-datatable-introduction/

The official data.table FAQ: https://cran.r-project.org/web/packages/data.table/vignettes/datatable-faq.html

Q&A

Questions – Comments – Feedback?

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THANK YOU FOR LISTENING

Find out more

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