



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

Research Data Scotland

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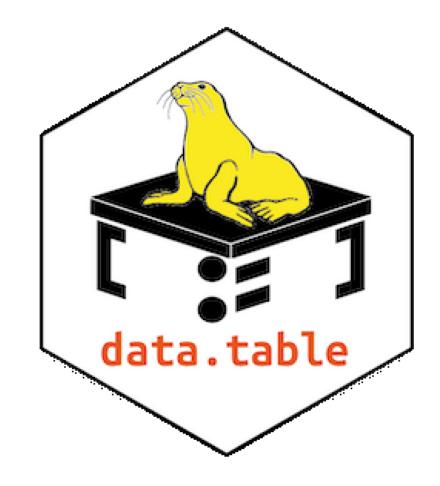


Outline

Introducing 'data.table'

Hands-on Session

Q&A



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



What will be faster: A Ferrari or a Honda?



What will be faster: A Ferrari or a Honda?

VS.



Photo by Stefano Probst on Unsplash



Photo by Brad armore on Unsplash



Apple-to-apple comparisons are required!

Task groupby join groupby2014 combine(groupby(DF, :id1), :v1 => sum...skipmissing => :v1) 0.5 GB 50 GB 5 GB DF.groupby('id1').agg(pl.sum('v1')).collect() 0.11: 0.05 basic questions DF.groupby('ld1', as_index=False, dropna=False).agg({'v1':'sum'}).compute() Input table: 1,000,000,000 rows x 9 columns (50 GB) **1**0.12: 0.10 DT[, .(v1=sum(v1, na.rm=TRUE)), by=id1] Polars 2021-06-30 8.8.0 143s data.table 0.16: 0.15 data.table 1.14.1 2021-06-30 155s SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1 DataFrames.jl 1.1.1 2021-05-15 200s 0.21; 0.16 256s SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1 ClickHouse 21.3.2.5 2021-05-12 clickhouse 0.13: 0.24 cuDF* 0.19.2 2021-05-31 492s DT[:, {'v1': sum(f.v1)}, by(f.id1)] 568s pydatatable 3.1.2 2021-05-31 spark 0.65: 0.67 2021-06-30 730s (py)datatable 1.0.0a0 SELECT id1, sum(v1) AS v1 FROM tbl GROUP BY id1 duckdb dplyr 1.0.7 2021-06-20 internal error 4.34; 0.06 DF %>% group_by(id1) %>% summarise(v1=sum(v1, na.rm=TRUE)) 1.2.5 2021-06-30 out of memory pandas dask 2021.04.1 2021-05-09 out of memory DF.groupby('id1', as_index=False, sort=False, observed=True, dropna=False).agg({'v1':'sum'}) 2021-05-31 internal error Arrow 4.0.1 First time out of memory DuckDB* 0.2.7 2021-06-15 DF.groupby('Id1', dropna=False, observed=True).agg({'v1':'sum'}).compute() Second time Modin see README pending AT %>% group_by(id1) %>% summarise(v1=sum(v1, na.rm=TRUE)) Minutes 0.5 1.5 2.5 3.0 1.0 2.0

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

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



Scene Setting

- 1) Routinely collected data has always been large and will only get larger (e.g. highdimensional 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)



"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 (\rightarrow even more time ...)



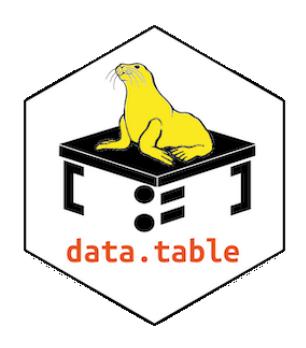
"Standard" R's limitations vs. data.table

- 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 (\rightarrow 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 (\rightarrow even more time ...) data.table has short and expressive code, similar to high-level programming languages



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/



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



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] \rightarrow subset where sex is "Male", then create V2...
data[sex == "Male", .(V2 = max(V1))] \rightarrow subset where sex is "Male", then return a new variable
data[, .(V2 = max(V1)), by = c("sex")] \rightarrow no subset, return new variable by group ("sex" variable)
```



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")]



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



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?



THANK YOU FOR LISTENING

Find out more

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