Overlap Death Match!

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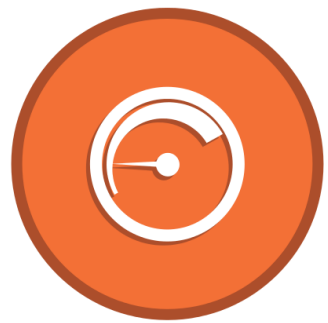
VS

Bioconductor

VS



data.table

12 February 2015

The contenders

Round 1: timings on genomic data

Round 2: accuracy on genomic data

And the champion is...

Google Summer of Code

Brief history of statistical computing

1957 FORTRAN by John Backus (IBM).

1972 C by Dennis Ritchie (Bell Labs).

1976 S by John M Chambers (Bell Labs).

1983 C++ by Bjarne Stroustrup (Bell Labs).

1993 S exclusively licensed to StatSci/MathSoft.
R by Ross Ihaka and Robert Gentleman
(Univ Auckland, New Zealand).

1998 Association of Computing Machinery Software System award to John M Chambers for "the S system, which has forever altered the way people analyze, visualize, and manipulate data."

Source: Wikipedia, R-FAQ.

R = interactive, graphical, programming with data

What is R? (Source: R-FAQ)
"R is a system for statistical computation and graphics. It consists of a language plus a run-time environment with graphics, a debugger, access to certain system functions, and the ability to run programs stored in script files."

interactive	command line (versus compiled).
graphical	publication-quality plots.
programming with data	`data.frame` which represents a tabular data set.

Selected Bioconductor project history

Version	Release	Packages	Depends	Firsts/notes
1.0	1 May 2001	15	R 1.5	
2.3	22 Oct 2008	294	R 2.8	IRanges
2.5	28 Oct 2009	352	R 2.10	findOverlaps
2.6	23 Apr 2010	389	R 2.11	GenomicRanges
3.0	14 Oct 2014	934	R 3.1	TESTED

Bioconductor = R packages with compiled C code.

Source: Wikipedia "Bioconductor," archived packages e.g. `http://www.bioconductor.org/packages/2.5`

Selected bedtools project history

```
VERSION 1.1, 04/23/2009. Initial release.
```

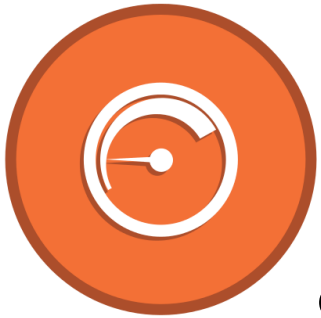
BEDTools: a flexible suite of utilities for comparing genomic features. Bioinformatics (2010).

```
Version 2.14.1-3 (2-Nov-2011)
         ...
         2.14.3-1                    TESTED ubuntu
         ...
Version 2.17.0   (3-Nov-2012)   TESTED guillimin
         ...
Version 2.22.1   (1 Jan 2015)   TESTED github
```

= command line C++ program.

Source: bedtools `RELEASE_HISTORY` file.

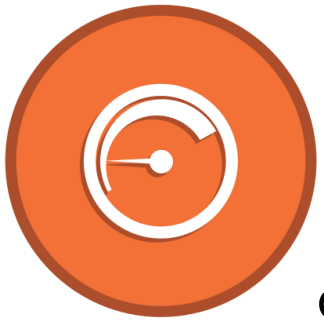
data.table is “just like a data.frame”



data.table = an R package with compiled C code.

```
Version: 1.0, 2006-04-12

Author: Matt Dowle

Title: Just like a data.frame but without rownames,
 up to 10 times faster, up to 10 times less memory
```

data.table is an "extension of data.frame"



data.table = an R package with compiled C code.

```
Version: 1.9.4, 2014-10-02

Author: M Dowle, T Short, S Lianoglou, A Srinivasan
 with contributions from R Saporta, E Antonyan

Title: Extension of data.frame

Description: Fast aggregation of large data
 (e.g. 100GB in RAM), fast ordered joins,
 fast add/modify/delete of columns
 by group using no copies at all,
 list columns and a fast file reader (fread)...
```

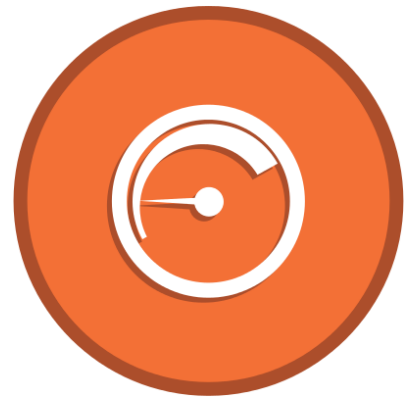
data.table supports overlap joins

data.table/README.md

```
Changes in v1.9.4 (on CRAN 2 Oct 2014)
NEW FEATURES
...
Overlap joins (#528) is now here, finally!!

Except for type="equal" and maxgap and minoverlap
arguments, everything else is implemented.

Check out ?foverlaps and the examples there on its usage.

This is a major feature addition to data.table.
```

https://github.com/Rdatatable/data.table/wiki/talks/EARL2014_OverlapRangeJoin_Arun.pdf

Summary of contenders, demo



		Bioconductor	data.table
Since	2009	2009	2014
Language	C++	R/C	R/C
Versions Tested	2.14.3	3.0	1.9.4
	2.17.0		
	2.22.1		

The contenders

Round 1: timings on genomic data

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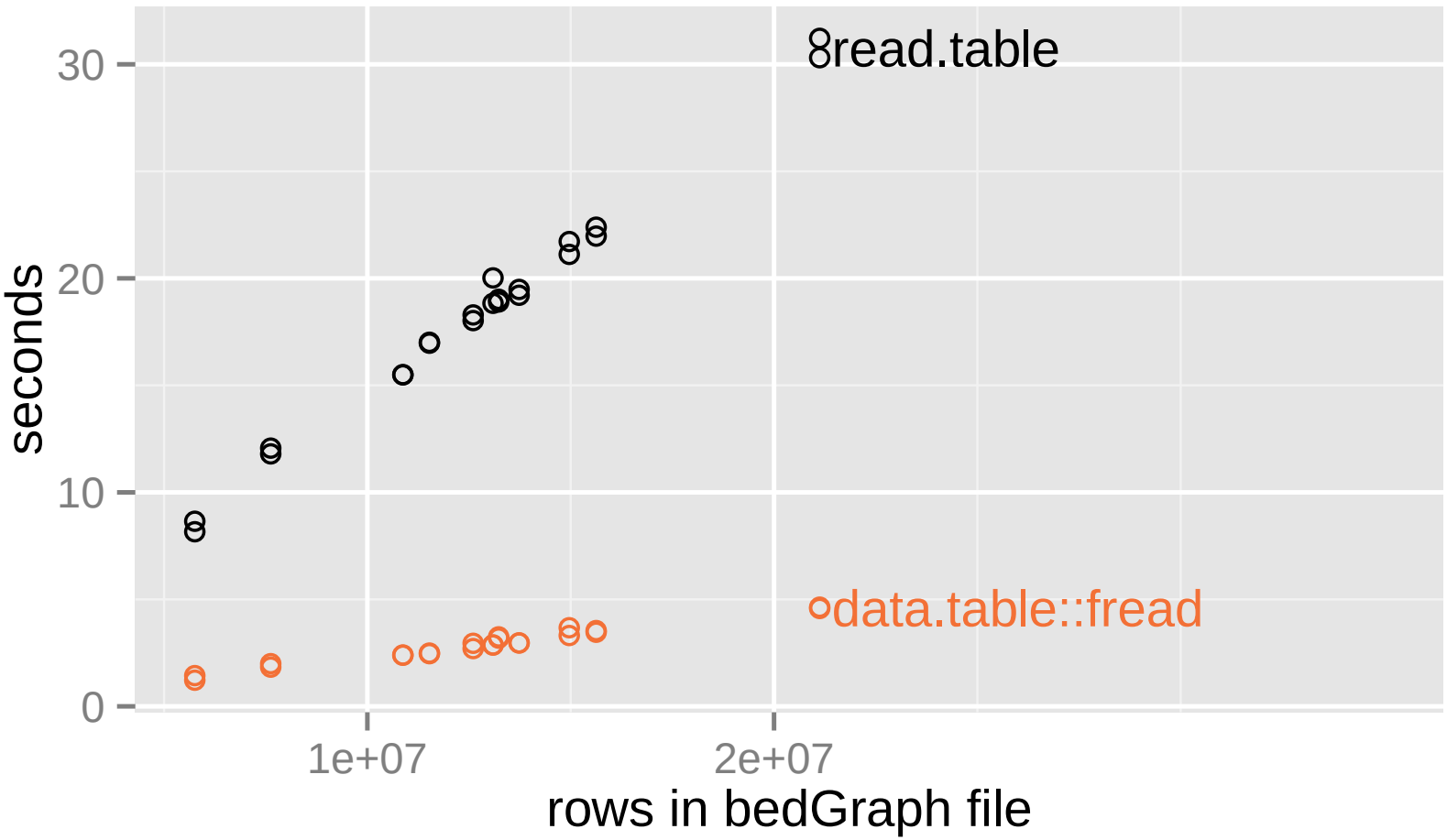
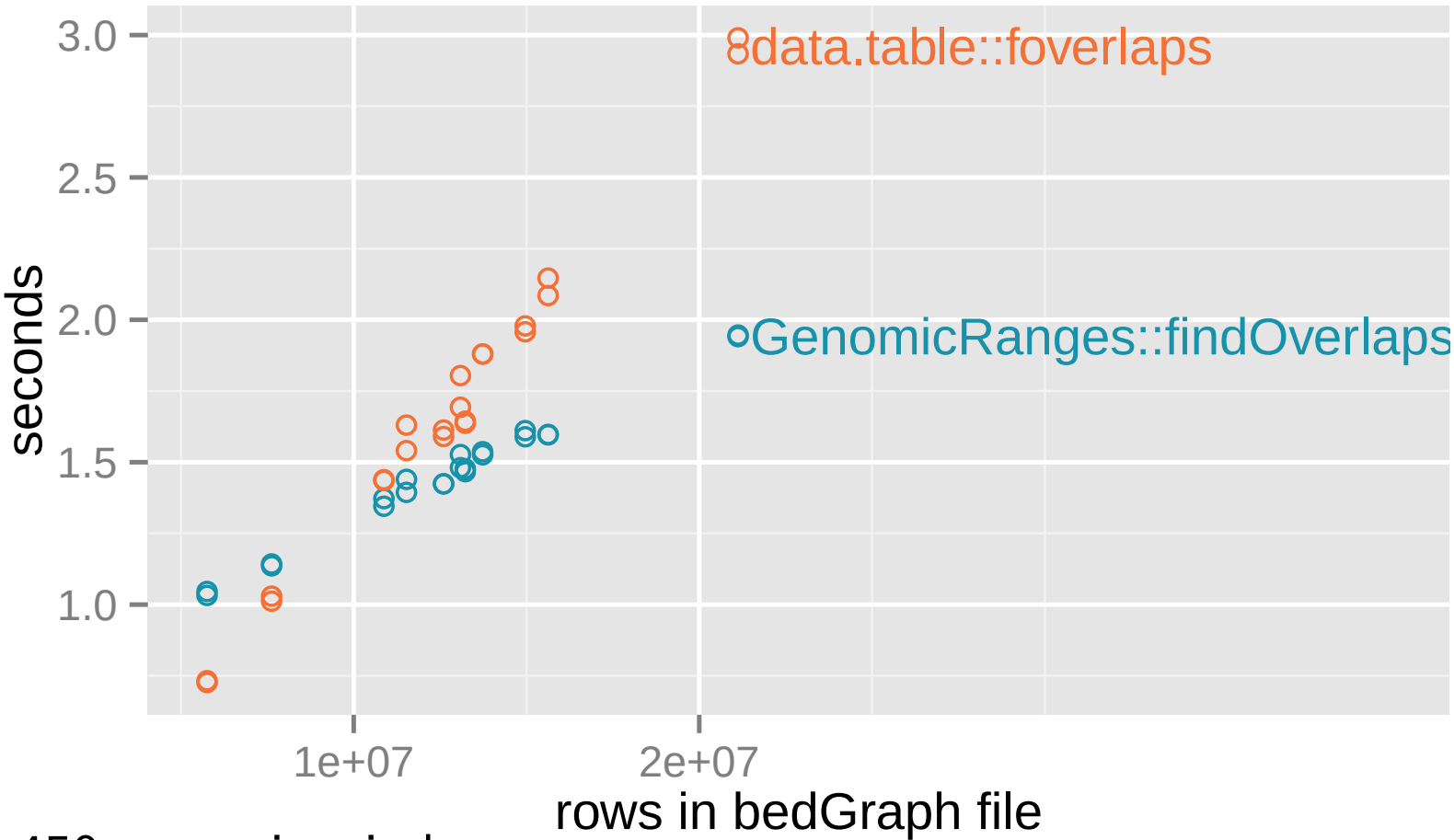
data.table::fread faster than read.table for bedGraph files



`read.table(file, sep=, colClasses=, nrows=)` vs `fread(file)`

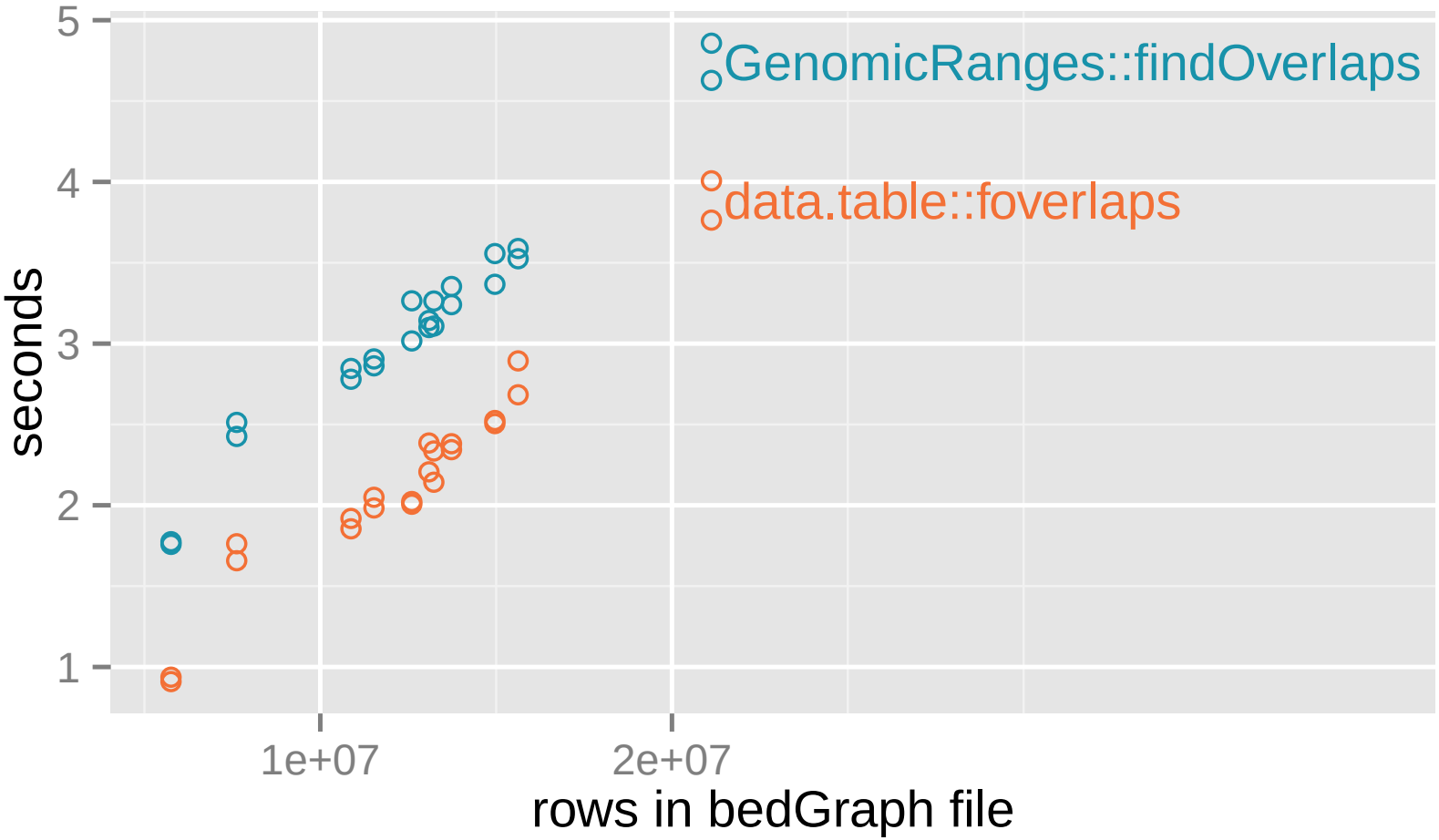
Only compute overlapping indices

```
GenomicRanges::findOverlaps(bedGraph.gr, windows.gr)
data.table::foverlaps(bedGraph.dt, windows.dt,
                      nomatch=0L, which=TRUE)
```



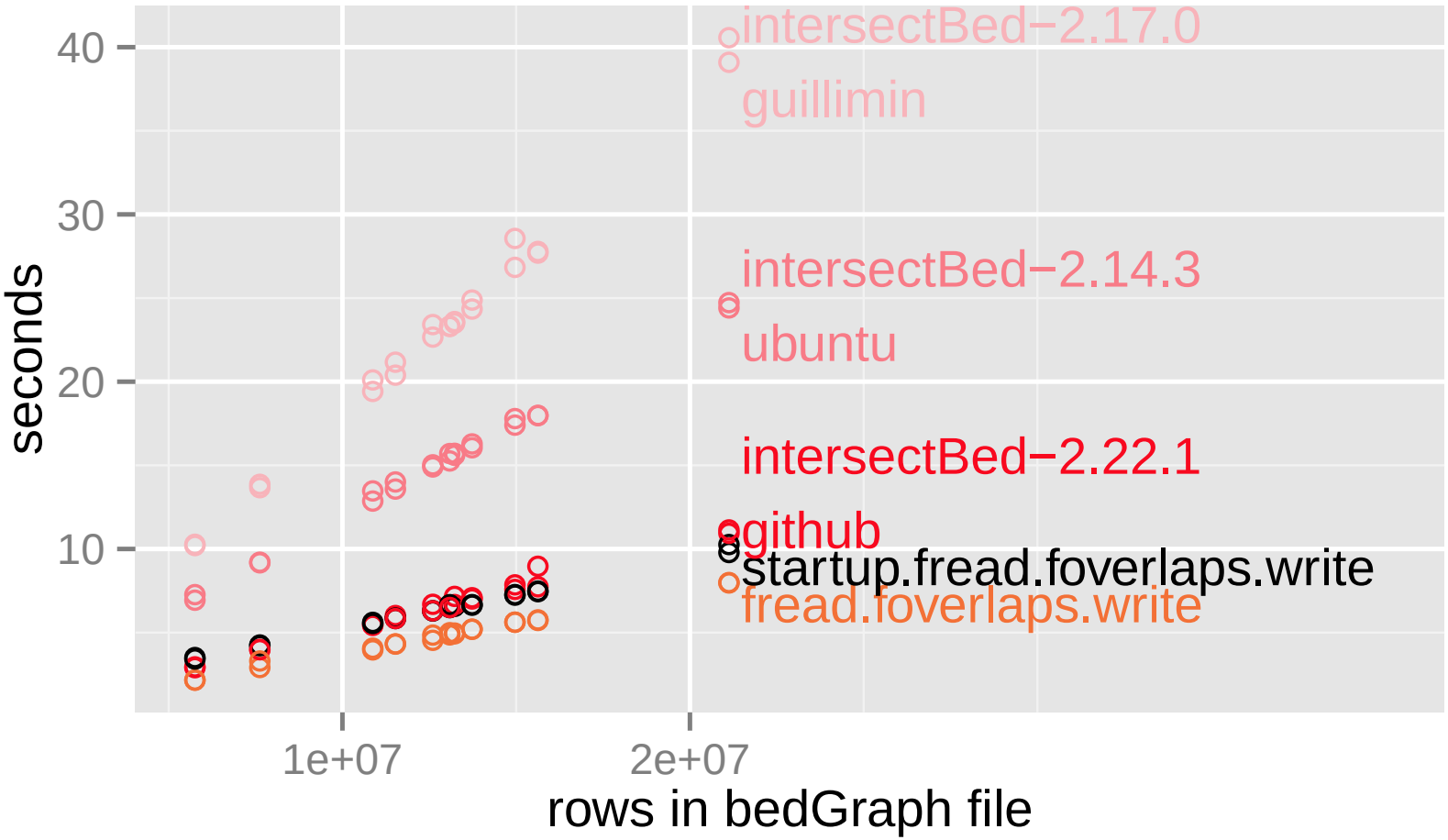
$\approx$ 450 genomic windows.

Start from data.frame, convert to GRanges/data.table, compute overlapping indices, select data



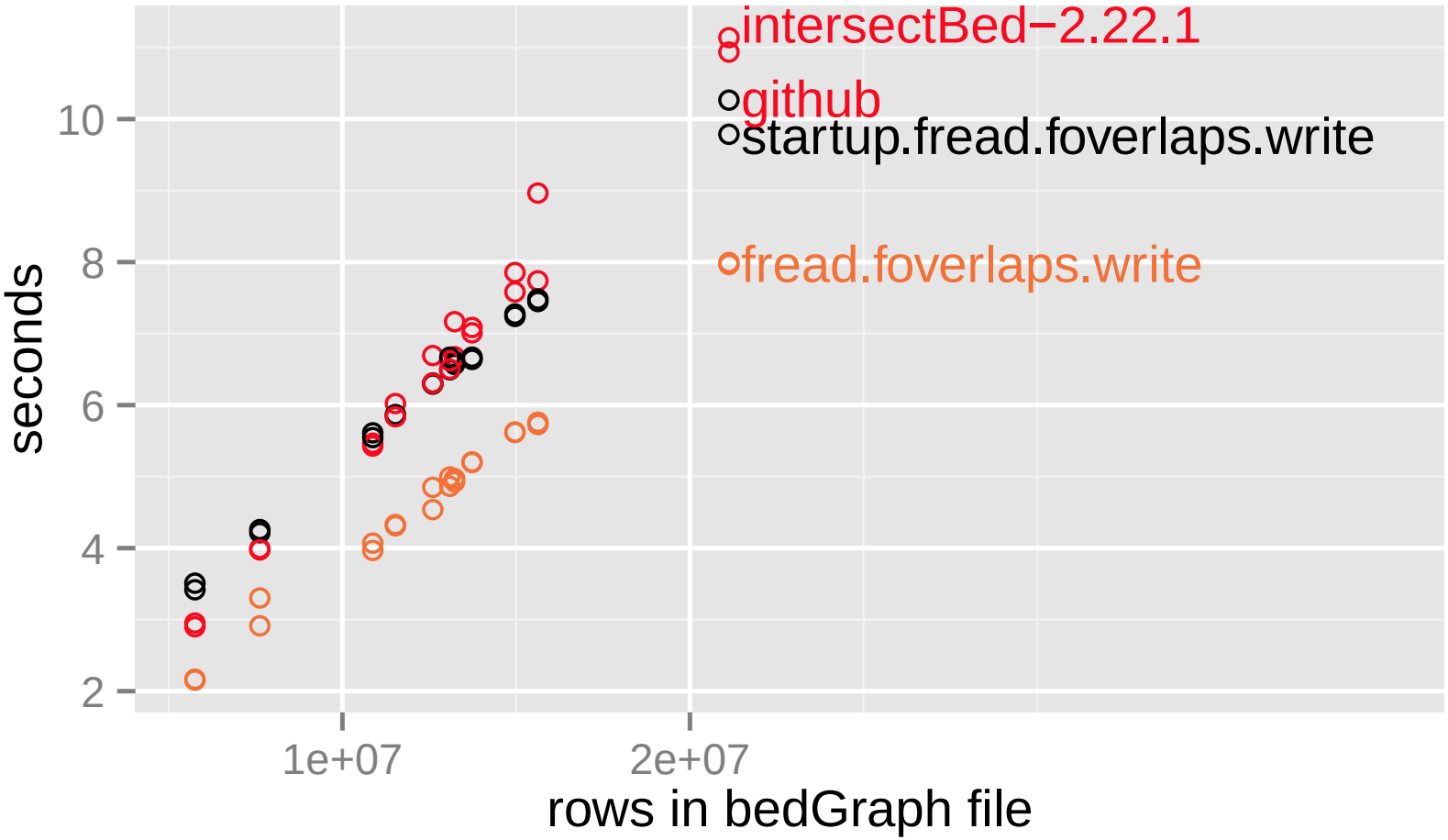
$\approx$ 450 genomic windows.

Read files, overlap, write file



$\approx$ 450 genomic windows.

Read files, overlap, write file



$\approx$ 450 genomic windows.

The contenders

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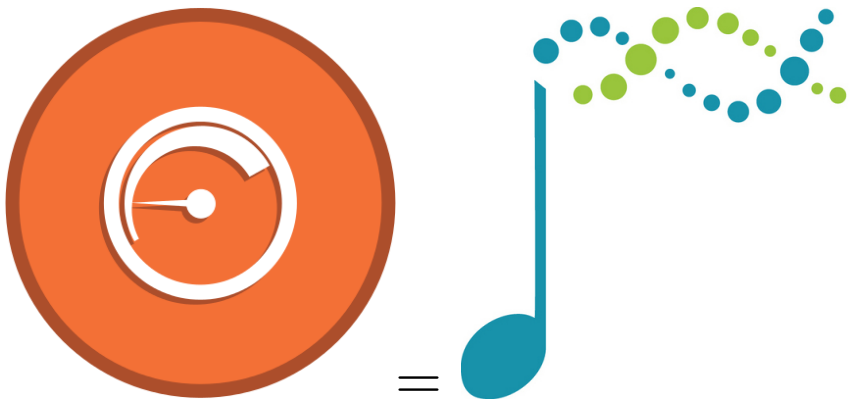
And the champion is...

Google Summer of Code

data.table::foverlaps always gives the same result as GenomicRanges::findOverlaps



... but are they correct?

Need chromStart+1 in R!

chipseq.bedGraph

```
chr1   0 200 0
chr1 200 300 1
```

chromStart	200	199	0	0
chromEnd	1000	1000	200	201
expected	1	0,1	0	0,1
findOverlaps	incorrect	ok	incorrect	ok
findOverlaps+1	ok	ok	ok	ok
foverlaps	incorrect	ok	incorrect	ok
foverlaps+1	ok	ok	ok	ok
intersectBed-2.22.1	ok	ok	ok	ok

The contenders

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All packages have similar speed, accuracy

Caveats:

- need most recent versions!
- need chromStart+1 in R!

Bonus points

+1 to

- **bedtools** for binary files (BAM).
- **data.table** for `fread`
  (read text files faster than `read.table`).
- **bedtools** and **GenomicRanges::findOverlaps** for
  -f/minoverlap
  (not yet implemented in `data.table::foverlaps`).
- **GenomicRanges::findOverlaps** for maxgap
  (not yet implemented in `data.table::foverlaps`).
- **bedtools** for native support for 0-based chromStart of bed/bedGraph files (need to use chromStart+1 in R).

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Google Summer of Code

Google Summer of Code (GSOC)

Student gets $5000 for writing open source code for 3 months.

Feb	**Admins** for open source organizations e.g. R, Bioconductor apply to Google.
Mar	**Mentors** suggest projects for each org. **Students** submit project proposals to Google. Google gives funding for n students to an org.
April	The top n students get $500 and begin coding.
July	Midterm evaluation, pass = $2250.
Aug	Final evaluation, pass = $2250.
November	Orgs get $500/student mentored.

I have participated as an **admin** and **mentor** for the R project.

What makes a good GSOC project?

Coding projects should:

- Result in free/open-source software.
- Be 3 months of full time work for a student.
- Include writing documentation and tests.
- Not include original research.

Examples:

- Louis/Mathieu can be **admins** for MUGQIC org.
- Warren/Stephan can be **mentors** for a project to write a new R package for methylation analysis.
- Robert/Dan can be **mentors** for a project to implement new features in Gemini.
- Any undergrad/master/PhD candidates (at McGill or not) can be **students**.

Thanks for your attention!

Any questions? toby.hocking@mail.mcgill.ca

Source code for benchmarks is at
https://github.com/tdhock/datatable-foverlaps

old intersectBed -sorted is much slower

"-sorted Invoke a memory-efficient algorithm for very large files."
Version: 2.14.3-1

```
$ time intersectBed -a windows.bed \
 -b chip-seq.bedGraph -sorted > overlap.bedGraph
real 154m10.653s
user 153m2.188s
sys  0m20.204s

$ time intersectBed -a windows.bed \
 -b chip-seq.bedGraph > overlap.bedGraph
real 0m8.733s
user 0m7.932s
sys  0m0.728s
```