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PyRanges paper supplementaries

This document shows the time and memory usage for all non-basic functions in the ecosystem of PyRanges libraries (PyRanges, PyRles and NCLS). They are compared against their equivalents in Python and R, respectively. The basic PyRanges functionality is compared against R Bioconductor's GenomicRanges and pybedtools. The PyRles-functionality is compared against R Bioconductor's S4Vectors. The NCLS is compared against the intervaltree in the Python bx-python library. For each function the equivalent code from each library is shown.

unary

PyRanges functionality that operates on a single PyRanges object. These include functions to sort, cluster and convert ranges into run length encodings (RLE.)

Sort

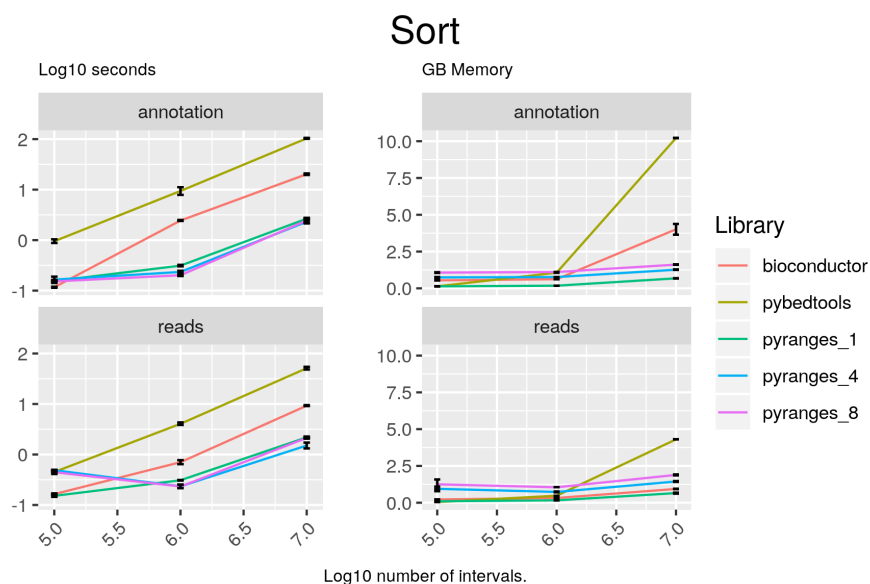


Figure 1: Sort the intervals on Start and End. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr.sort()
```

bioconductor

```
result = sortSeqlevels(gr)  
result = sort(result)
```

pybedtools

```
result = pbl.sort()
```

Cluster

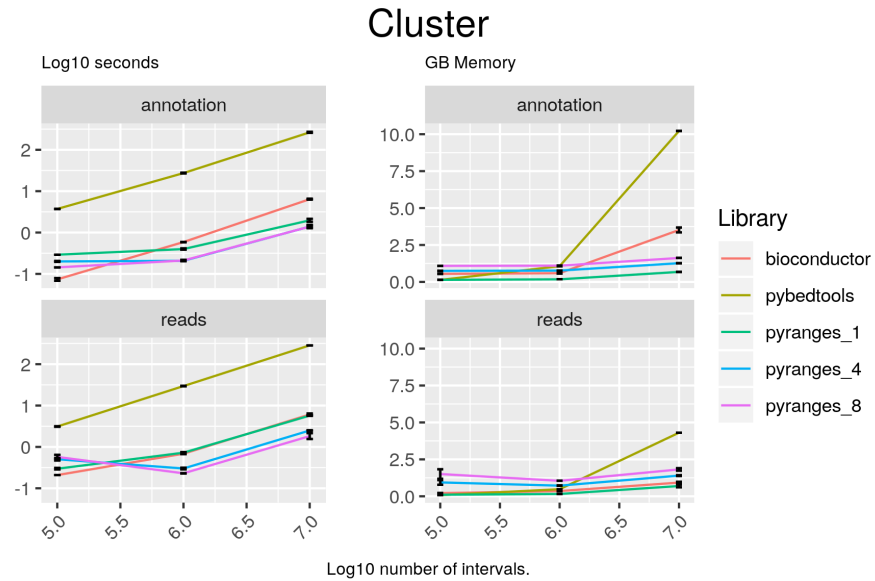


Figure 2: Order intervals by position and merge those overlapping. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr.cluster(strand="same")
```

bioconductor

```
result = reduce(gr)
```

pybedtools

```
if extension == "gtf":  
    cols_to_keep = [4, 5, 7]
```

```
elif extension == "bed":  
    cols_to_keep = [4, 5, 6]  
  
    plus = pb1.sort().merge(S="+", c=cols_to_keep, o="first")  
    minus = pb1.sort().merge(S="-", c=cols_to_keep, o="first")  
    result = plus.cat(minus, s=True, c=[4, 5, 6], o="first")
```

Genomicrange_to_coverage

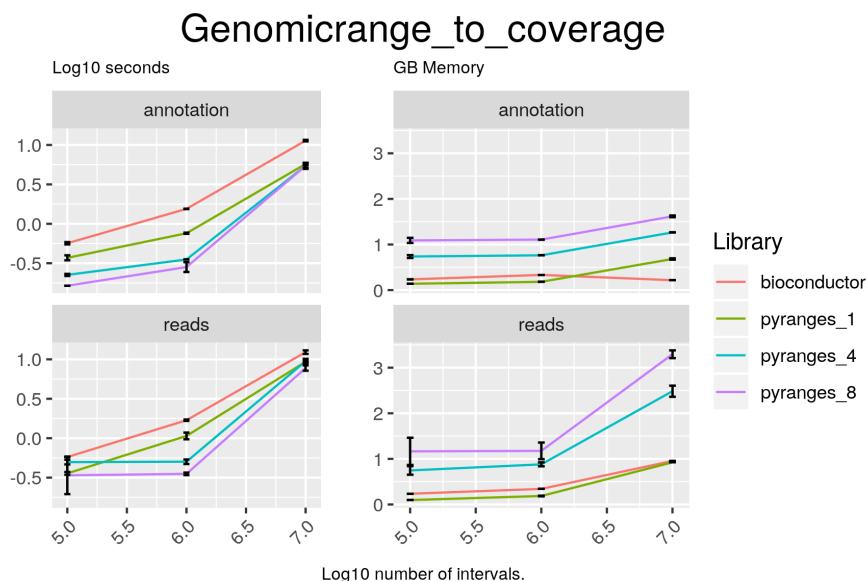


Figure 3: Turn ranges into run length encodings. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr.coverage(strand="same")
```

bioconductor

```
plus = coverage(gr[gr@strand == "+"])
minus = coverage(gr[gr@strand == "-"])
result = c(plus, minus)
```

binary

PyRanges functionality that operates on pairs of PyRanges. These functions include functions to find the nearest intervals, find the intersecting intervals, join granges on overlap, set intersect/union and subtract one PyRanges object from another.

Overlap

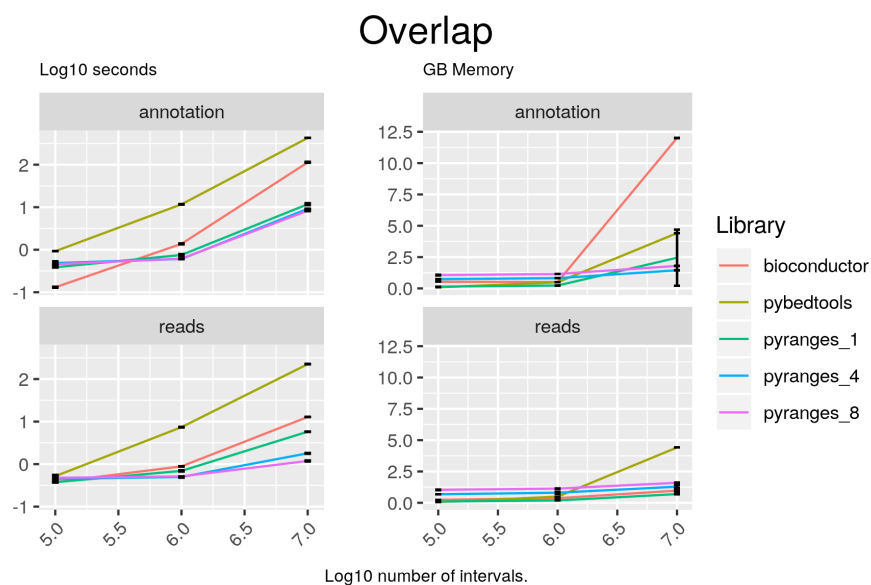


Figure 4: Find the intervals in A overlapping at least one of the intervals in B. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.overlap(gr, strandedness="same")
```

bioconductor

```
result = findOverlapPairs(gr2, gr1, ignore.strand = FALSE)
result = first(result)
```

pybedtools

```
result = pb2.intersect(pb1, s=True, wa=True)
```


Intersect

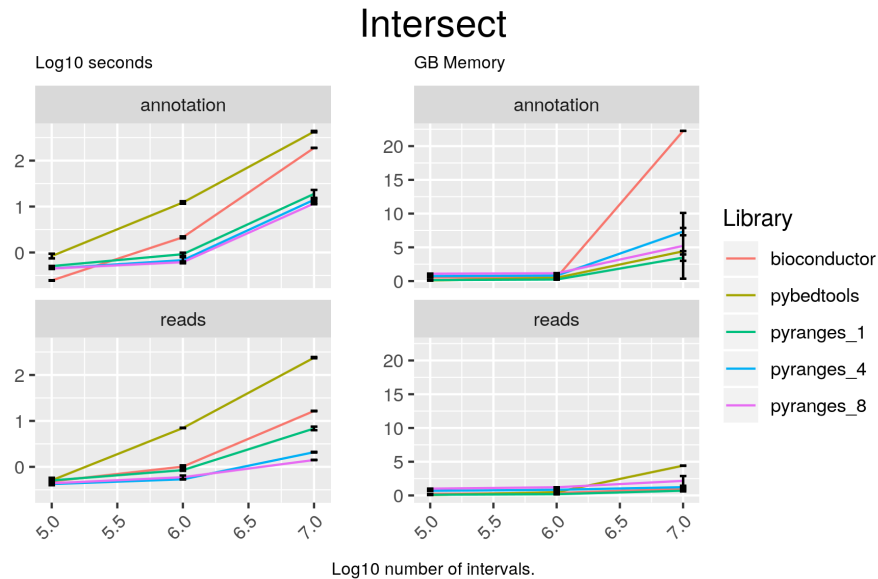


Figure 5: Find overlapping intervals in both datasets. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.intersect(gr, strandedness="same")
```

bioconductor

```
pairs = findOverlapPairs(gr2, gr1, ignore.strand = FALSE)
result = pintersect(pairs, ignore.strand = FALSE)
result = result[mcols(result)$hit == TRUE]
```

pybedtools

```
result = pb2.intersect(pb1, s=True)
```

Nearest

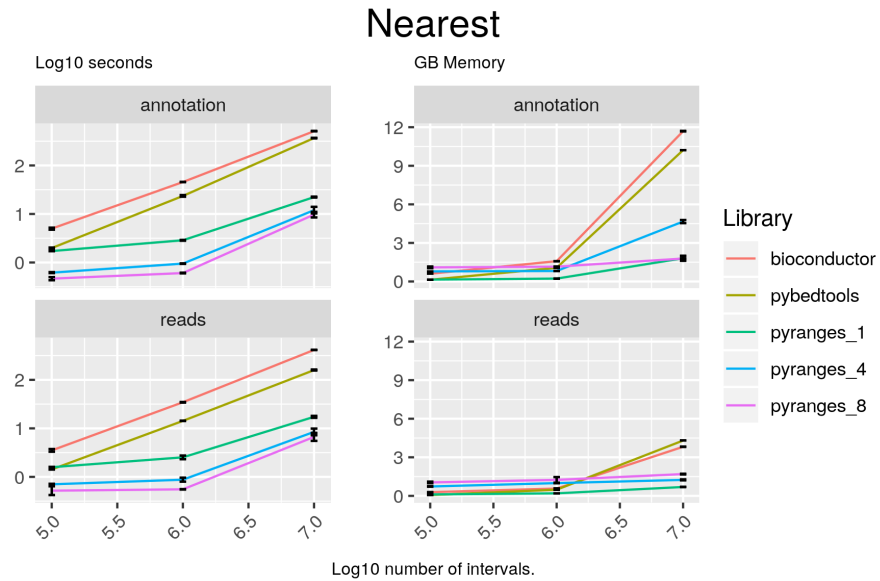


Figure 6: Find the intervals in B closest to those in A. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr.nearest(gr2, strandedness="same")
```

bioconductor

```
result = distanceToNearest(gr2, gr1, ignore.strand = FALSE, select="
  arbitrary")
subject = as.data.frame(gr1[subjectHits(result)])
colnames(subject) = paste0(colnames(subject), "_b")
query = as.data.frame(gr2[queryHits(result)])
df = merge(subject, query, by=0)
df = df[, -1]
df = merge(df, mcols(result)$distance, by=0)
```

```
df = df[, -1]  
result = makeGRangesFromDataFrame(df, keep.extra.columns=TRUE)
```

pybedtools

```
result = pb2.sort().closest(pb1.sort(), s=True, t="first", d=True)
```

Nearest_nonoverlapping

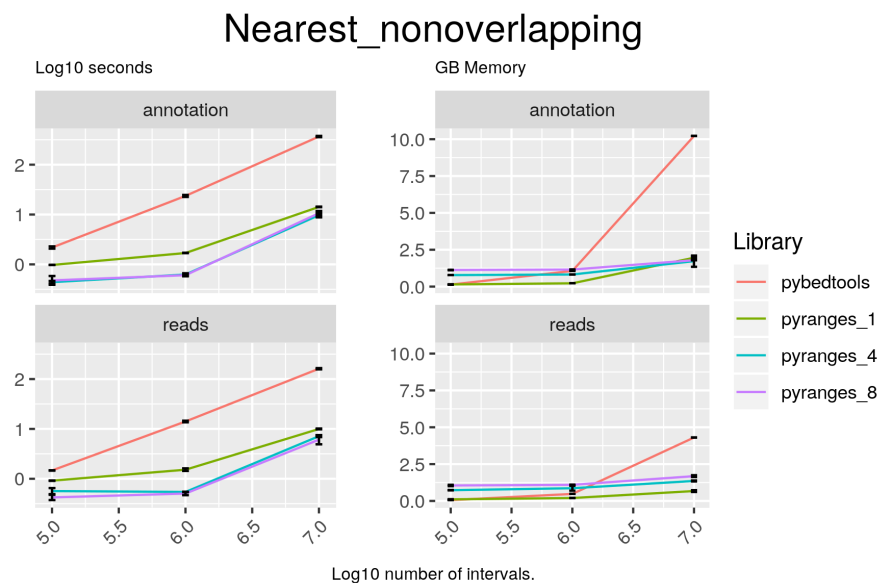


Figure 7: Find the non-overlapping intervals in B closest to those in A. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr.nearest(gr2, strandedness="same", overlap=False)
```

pybedtools

```
result = pb2.sort().closest(pb1.sort(), s=True, t="first", io=True, d=True)
```

Subtract

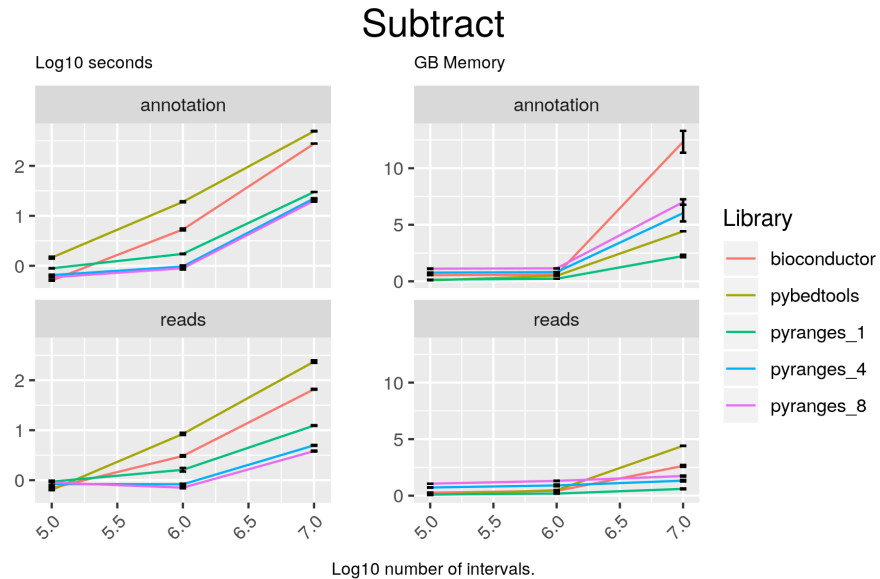


Figure 8: Remove all intervals in B from those in A. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.subtract(gr, strandedness="same")
```

bioconductor

```
hits <- findOverlaps(gr2, gr1, ignore.strand = FALSE)
toSubtract <- reduce(extractList(gr1, as(hits, "List")),
  ignore.strand = FALSE)
ans <- unlist(psetdiff(gr2, toSubtract, ignore.strand = FALSE))
result <- subset(ans, width(ans) > 0L)
```

pybedtools

```
result = pb2.subtract(pb1, s=True)
```

Set_intersect

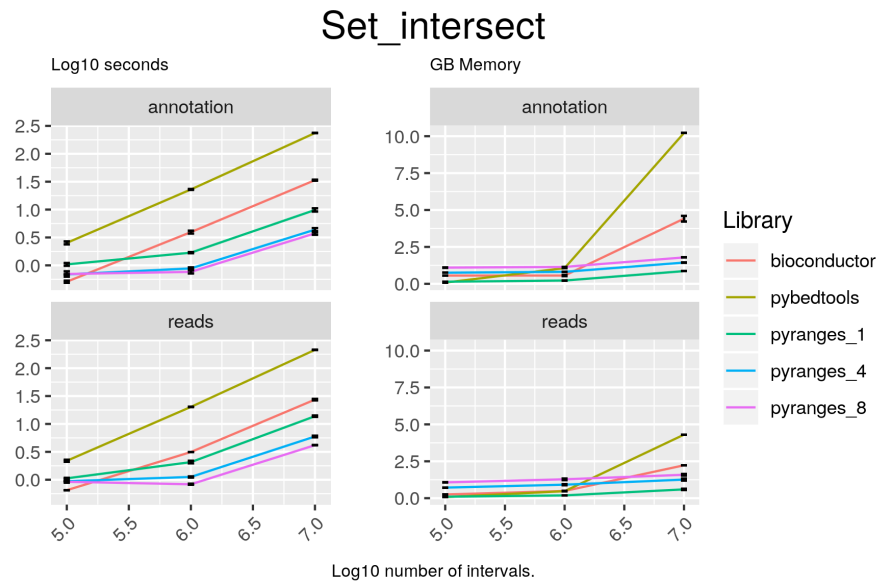


Figure 9: Intersect the set union of the ranges. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.set_intersect(gr, strandedness="same")
```

bioconductor

```
result = intersect(gr2, gr1)
```

pybedtools

```
sc = pb1.sort().merge(s=True, c=[4, 5, 6], o="first")
```

```
if extension == "gtf":
    cols_to_keep = [4, 5, 7]
elif extension == "bed":
    cols_to_keep = [4, 5, 6]

sb = pb2.sort().merge(s=True, c=cols_to_keep, o="first ")
result = sc.intersect(sb, s=True)
```


Set_union

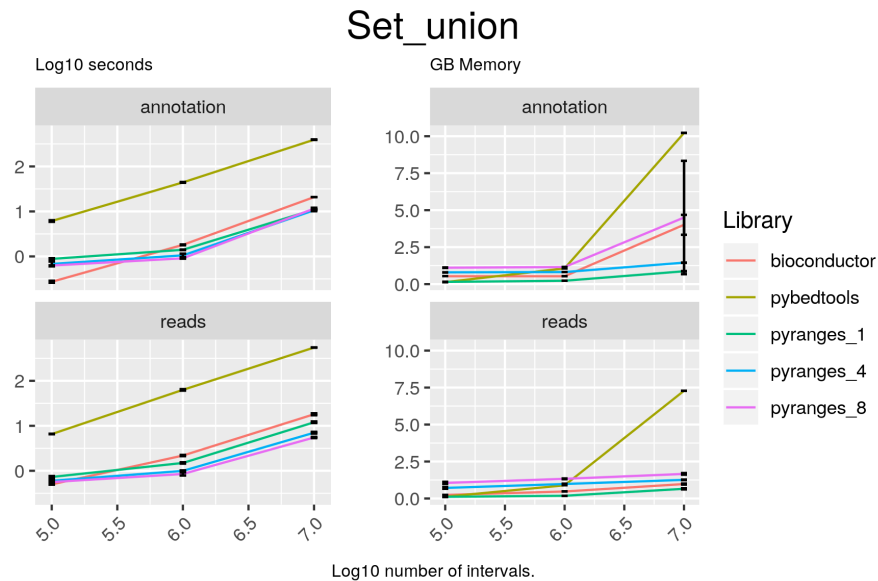


Figure 10: Concatenate the datasets and cluster them afterwards. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.set_union(gr, strandedness="same")
```

bioconductor

```
result = union(gr1, gr2)
```

pybedtools

```
sc = pb1.sort().merge(s=True, c=[4, 5, 6], o="first")
```

```
if extension == "gtf":
    cols_to_keep = [4, 5, 7]
elif extension == "bed":
    cols_to_keep = [4, 5, 6]

sb = pb2.sort().merge(s=True, c=cols_to_keep, o="first")
catted = sc.cat(sb, s=True, c=[4, 5, 6], o="first").sort()
result = catted.merge(s=True, c=[4, 5, 6], o="first")
```

Jaccard

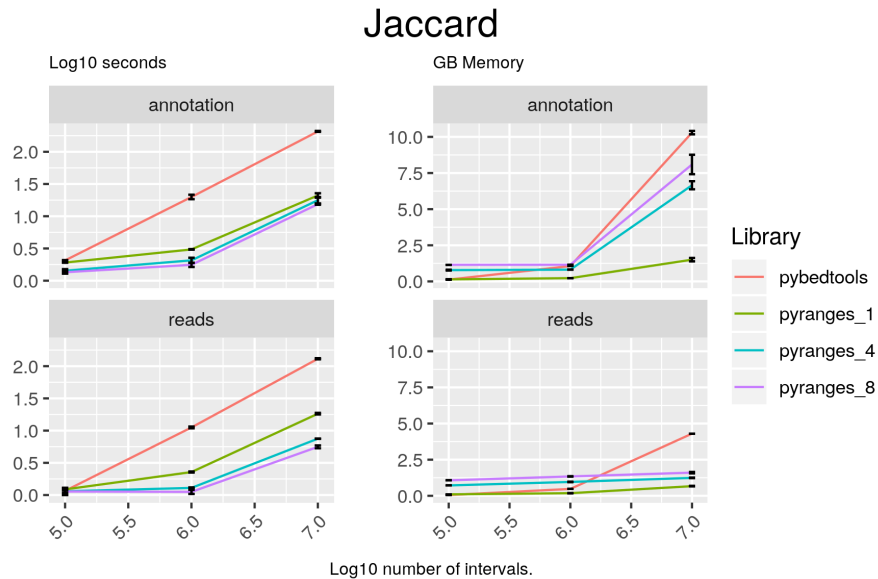


Figure 11: Find similarity between sets based on intersections. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.stats.jaccard(gr)
```

pybedtools

```
result = pb2.sort().jaccard(pb1.sort())
```

Join

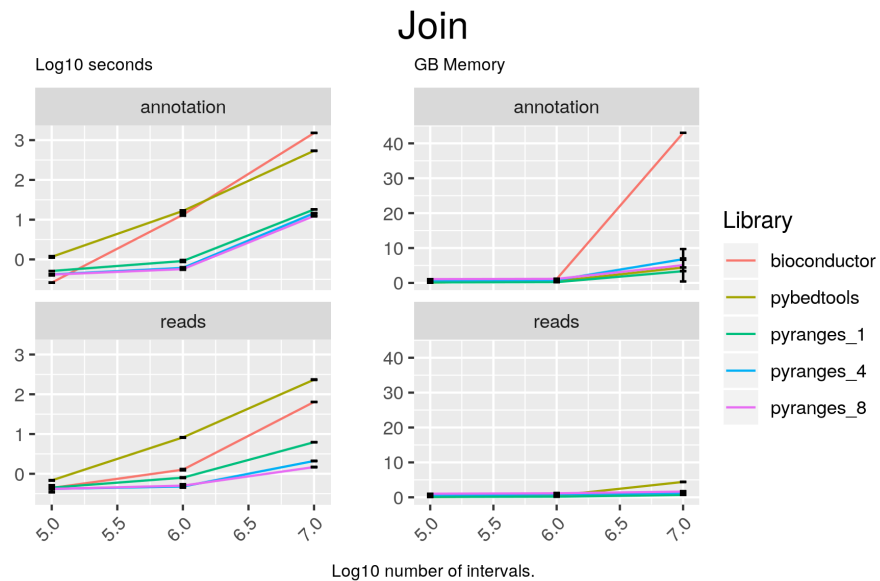


Figure 12: Find the overlapping intervals and combine their data. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = gr2.join(gr, strandedness="same")
```

pybedtools

```
result = pb2.intersect(pb1, wao=True, s=True)
```

bioconductor

```
result <- findOverlapPairs(gr1, gr2, ignore.strand = FALSE)
df1 = as.data.frame(first(result))
```

```
df2 = as.data.frame(second(result))
colnames(df2) = paste0(colnames(df2), "_b")
df = merge(df1, df2, by=0)
result = makeGRangesFromDataFrame(df, keep.extra.columns=TRUE)
```

rle

Arithmetic operations on RLEs. These include add, subtract, divide and multiply.

Rle_divide

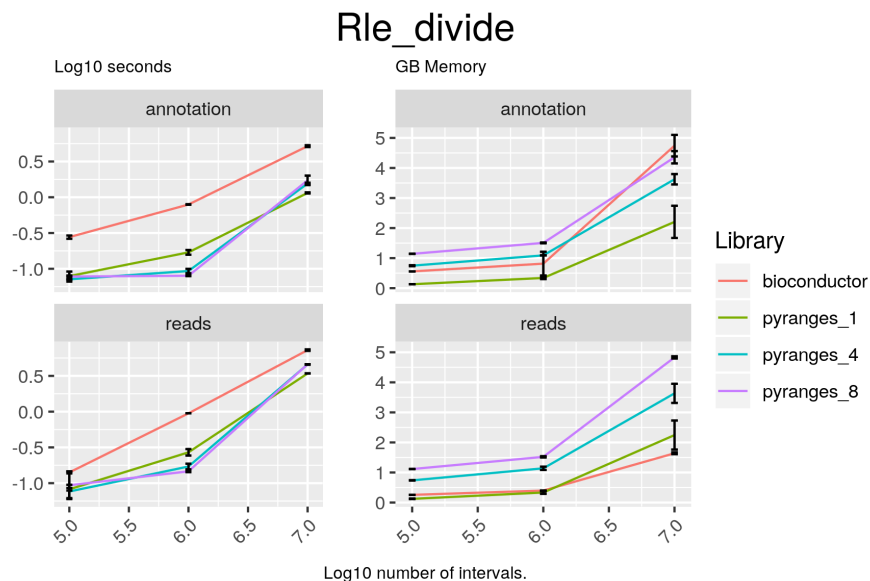


Figure 13: Divide one Rle object by another. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

bioconductor

```
result = c(c1p / c2p, c1m / c2m)
```

pyranges

```
result = c1 / c2
```

Rle_add

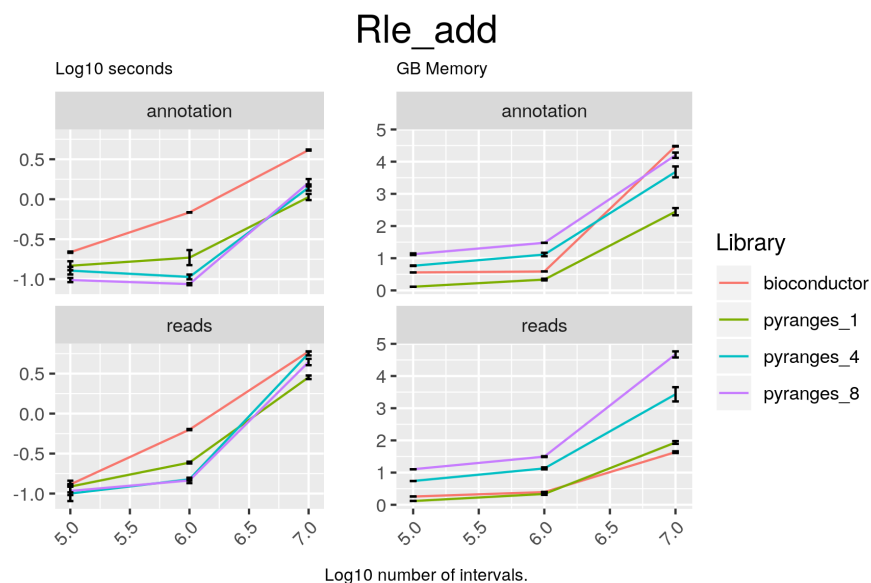


Figure 14: Add two Rle objects. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

bioconductor

```
result = c(c1p + c2p, c1m + c2m)
```

pyranges

```
result = c1 + c2
```

Rle_subtract

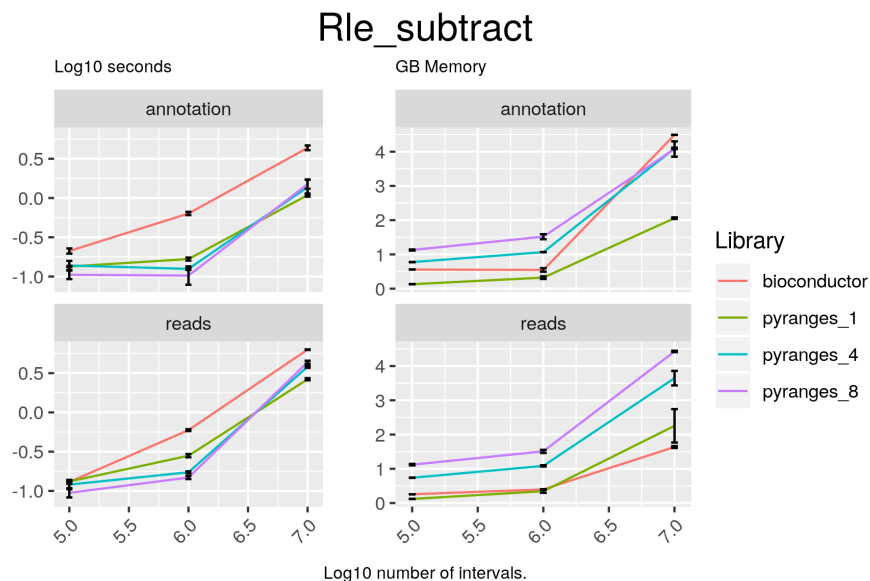


Figure 15: Subtract one Rle object from another. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

bioconductor

```
result = c(c1p - c2p, c1m - c2m)
```

pyranges

```
result = c1 - c2
```


Rle_multiply

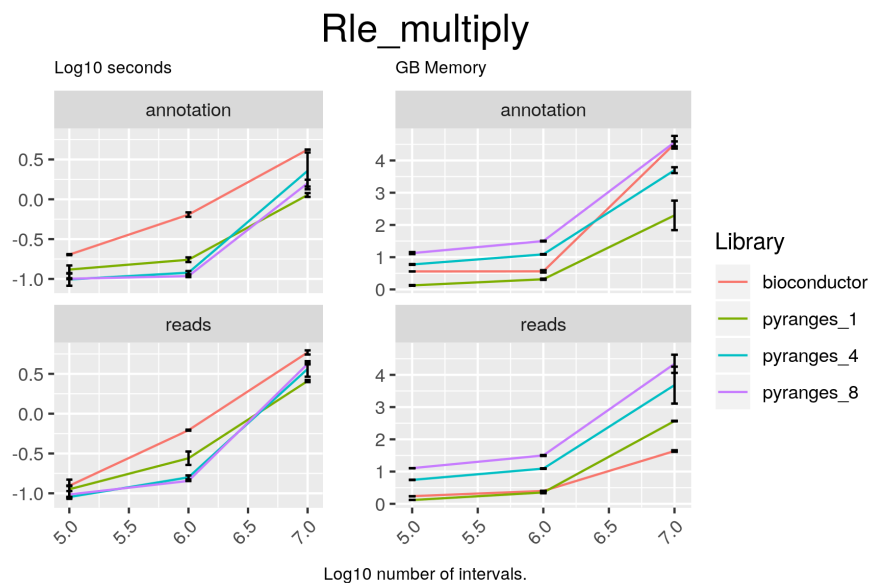


Figure 16: Multiply two Rle objects. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

bioconductor

```
result = c(c1p * c2p, c1m * c2m)
```

pyranges

```
result = c1 * c2
```

tree

Operations for building and finding overlaps using a tree.

Tree_build

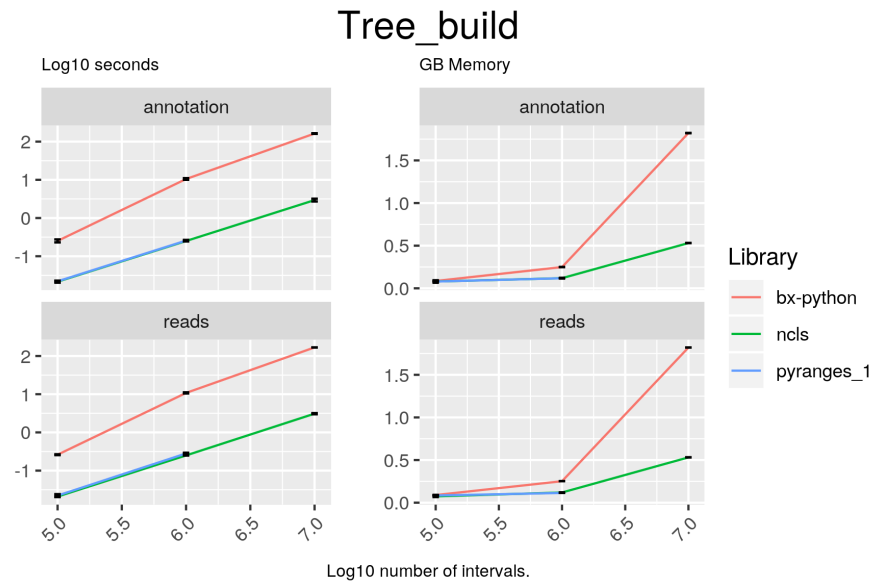


Figure 17: Create a tree from a collection of intervals. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

ncls

```
tree = NCLS(df2.Start.values, df2.End.values, df2.index.values)
```

bx-python

```
tree = IntervalTree()
for start_, end_ in zip(df2.Start, df2.End):
    tree.add(start_, end_)
```

Tree_overlap

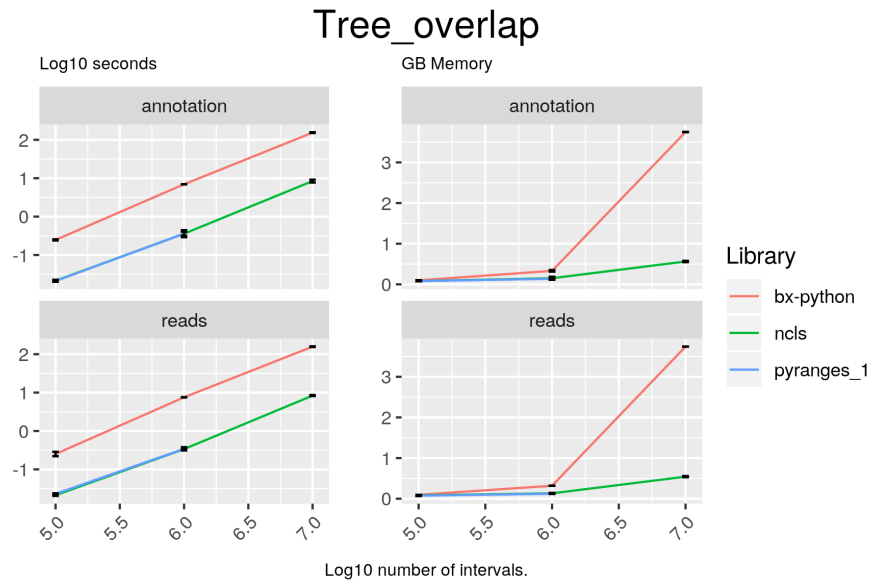


Figure 18: Search in a tree using a collection of intervals. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

ncls

```
result = tree.all_overlaps_self(df1.Start.values, df1.End.values, df1.index.values)
result = df2.iloc[result]
```

bx-python

```
result = []
for start_, end_ in zip(df1.Start, df1.End):
    result.append(tree.search(start_, end_))
```

io

Functions to read files into PyRanges.

Read_bed

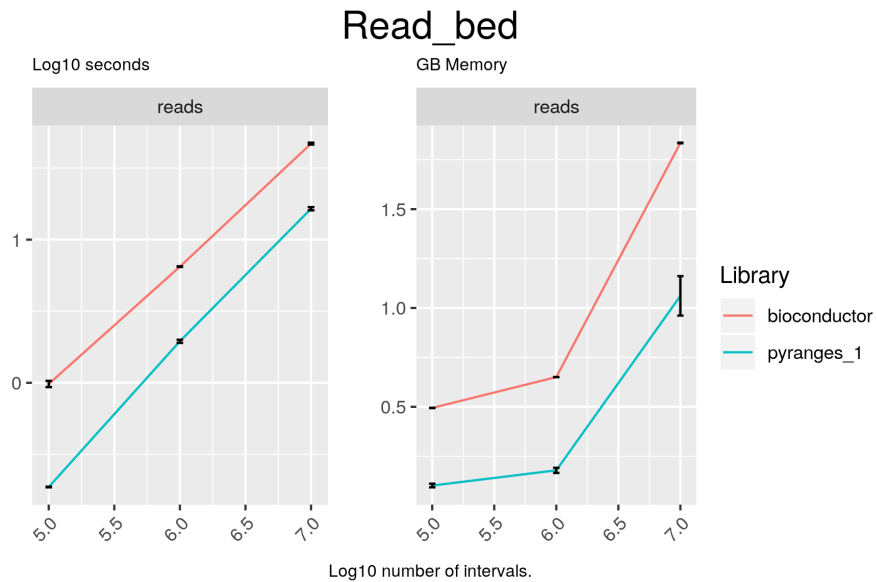


Figure 19: Read a bed file into a GenomicRanges object. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = pr.read_bed(f)
```

bioconductor

```
result = import(file)
```

Read_bam

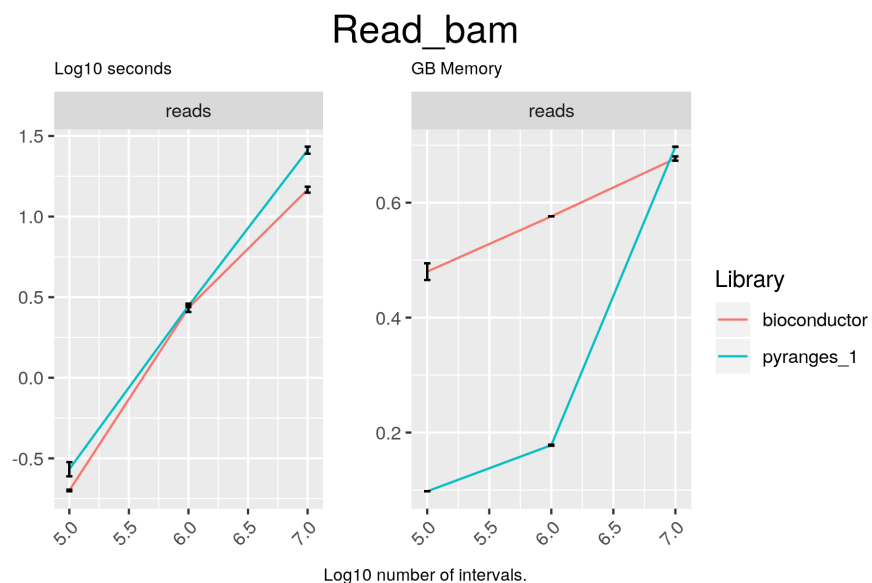


Figure 20: Read a bam file into a GenomicRanges object. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = pr.read_bam(f)
```

bioconductor

```
result = import(file)
```

Read_gtf

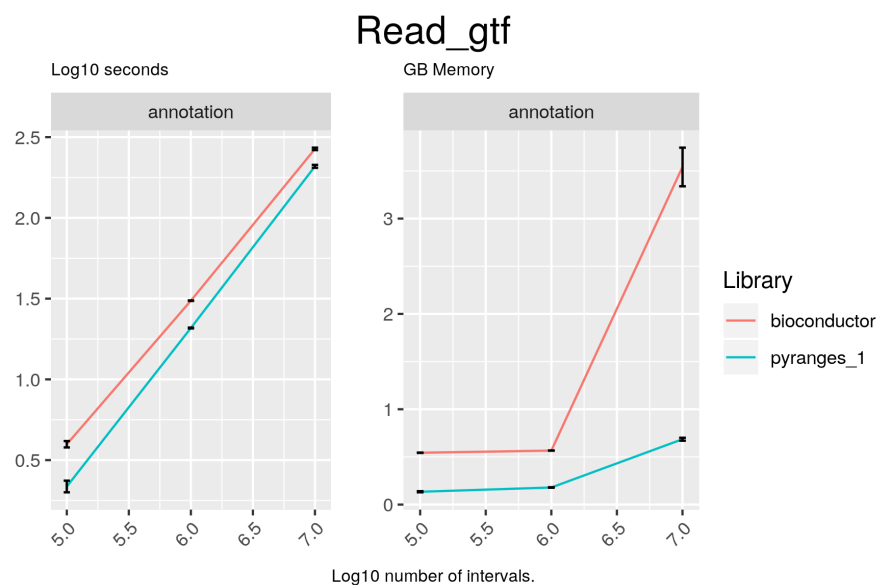


Figure 21: Read a gtf file into a GenomicRanges object. Comparison of the running time and memory usage for PyRanges versus the equivalent libraries in R and/or Python. In the top row the results for GTF data, while the bottom row shows the results for BED data. The left column shows the time usage, while the right column shows the memory usage. Time is measured in log10 seconds, while memory is measured in GigaBytes (GB).

Code

pyranges

```
result = pr.read_gtf(f, annotation="ensembl")
```

bioconductor

```
result = import(file)
```