

Working with large arrays in R

A look at HDF5Array/RleArray/DelayedArray objects

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Bioconductor conference
Boston

July 2017

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1 Motivation and challenges

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R ordinary **matrix** or **array** is not suitable for big datasets:

- 10x Genomics dataset (single cell experiment): 30,000 genes \times 1.3 million cells = 36.5 billion values
- in an ordinary integer matrix \implies 136G in memory!

Need for alternative containers:

- but at the same time, the object should be (almost) as easy to manipulate as an ordinary matrix or array
- *standard R matrix/array API*: `dim`, `dimnames`, `t`, `is.na`, `==`, `+`, `log`, `cbind`, `max`, `sum`, `colSums`, etc...
- not limited to 2 dimensions \implies also support arrays of arbitrary number of dimensions

2 approaches: **in-memory data** vs **on-disk data**

In-memory data

- a $30k \times 1.3M$ matrix might still fit in memory if the data can be efficiently compressed
- example: sparse data (small percentage of nonzero values) \implies *sparse representation* (storage of nonzero values only)
- example: data with long runs of identical values \implies *RLE compression* (*Run Length Encoding*)
- choose the *smallest type* to store the values: raw (1 byte) < integer (4 bytes) < double (8 bytes)
- if using *RLE compression*:
 - choose the *best orientation* to store the values: *by row* or *by column* (one might give better compression than the other)
 - store the data by chunk \implies opportunity to pick up *best type* and *best orientation* on a chunk basis (instead of for the whole data)
- size of $30k \times 1.3M$ matrix in memory can be reduced from 136G to 16G!

Examples of in-memory containers

dgCMatrix container from the *Matrix* package:

- sparse matrix representation
- nonzero values stored as double

RleArray and **RleMatrix** containers from the *DelayedArray* package:

- use RLE compression
- arbitrary number of dimensions
- type of values: any R atomic type (integer, double, logical, complex, character, and raw)

On-disk data

However...

- if data is too big to fit in memory (even after compression) \implies must use *on-disk representation*
- challenge: should still be (almost) as easy to manipulate as an ordinary matrix! (*standard R matrix/array API*)

Examples of on-disk containers

Direct manipulation of an **HDF5 dataset** via the *rhdf5* API. Low level API!

HDF5Array and **HDF5Matrix** containers from the *HDF5Array* package:

Provide access to the HDF5 dataset via an API that mimics the standard R matrix/array API

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The "airway" dataset

```
library(airway)
data(airway)
m <- unname(assay(airway))
dim(m)

## [1] 64102      8

typeof(m)

## [1] "integer"
```

```
head(m, n=4)

##           [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
## [1,]    679   448   873   408 1138 1047  770  572
## [2,]      0     0     0     0     0     0     0     0
## [3,]    467   515   621   365   587   799   417   508
## [4,]    260   211   263   164   245   331   233   229

tail(m, n=4)

##           [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
## [64099,]      0     0     0     0     0     0     0     0
## [64100,]      0     0     0     0     0     0     0     0
## [64101,]      0     0     0     0     0     0     0     0
## [64102,]      0     0     0     0     0     0     0     0

sum(m != 0) / length(m)

## [1] 0.3863803
```

dgCMatrix vs RleMatrix vs HDF5Matrix

```
library(lobstr) # for obj_size()
obj_size(m)

## 2,052,136 B

library(Matrix)
obj_size(as(m, "dgCMatrix"))

## 2,379,248 B

library(DelayedArray)
obj_size(as(m, "RleMatrix"))

## 2,217,496 B

obj_size(as(t(m), "RleMatrix"))

## 1,743,608 B

library(HDF5Array)
obj_size(as(m, "HDF5Matrix"))

## 2,464 B
```

Some limitations of the sparse matrix implementation in the *Matrix* package:

- nonzero values always stored as `double`, the most memory consuming type
- number of nonzero values must be $< 2^{31}$
- limited to 2 dimensions: no support for arrays of arbitrary number of dimensions

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RleMatrix/RleArray and HDF5Matrix/HDF5Array provide:

- support all R atomic types
- no limits in size (but each dimension must be $< 2^{31}$)
- arbitrary number of dimensions

And also:

- **delayed operations**
- **block processing** (behind the scene)
- TODO: multicore block processing (sequential only at the moment)

Delayed operations

We start with HDF5Matrix object M:

```
M <- as(m, "HDF5Matrix")
M

## <64102 x 8> matrix of class HDF5Matrix and type "integer":
##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
## [1,] 679 448 873 408 1138 1047 770 572
## [2,]  0  0  0  0  0  0  0  0
## [3,] 467 515 621 365 587 799 417 508
## [4,] 260 211 263 164 245 331 233 229
## [5,]  60  55  40  35  78  63  76  60
## ...
## [64098,]  0  0  0  0  0  0  0  0
## [64099,]  0  0  0  0  0  0  0  0
## [64100,]  0  0  0  0  0  0  0  0
## [64101,]  0  0  0  0  0  0  0  0
## [64102,]  0  0  0  0  0  0  0  0
```

RleArray and HDF5Array objects

Subsetting is delayed:

```
M2 <- M[10:12, 1:5]
M2

## <3 x 5> matrix of class DelayedMatrix and type "integer"
##      [,1] [,2] [,3] [,4] [,5]
## [1,] 394  236  464  175  658
## [2,] 172  168  264  118  241
## [3,] 2112 1867  5137 2657 2735
```

```
seed(M2)

## An object of class "HDF5ArraySeed"
## Slot "filepath":
## [1] "D:/biocbuild/bbs-3.14-
bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00002.h5"
##
## Slot "name":
## [1] "/HDF5ArrayAUT000002"
##
## Slot "as_sparse":
## [1] FALSE
##
## Slot "type":
## [1] NA
##
## Slot "dim":
## [1] 64102      8
##
## Slot "chunkdim":
## [1] 64102      8
##
## Slot "first_val":
## [1] 679
```

RleArray and HDF5Array objects

Transposition is delayed:

```
M3 <- t(M2)
M3

## <5 x 3> matrix of class DelayedMatrix and type "integer"
##      [,1] [,2] [,3]
## [1,] 394  172 2112
## [2,] 236  168 1867
## [3,] 464  264 5137
## [4,] 175  118 2657
## [5,] 658  241 2735
```

```
seed(M3)

## An object of class "HDF5ArraySeed"
## Slot "filepath":
## [1] "D:/biocbuild/bbs-3.14-
bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00002.h5"
##
## Slot "name":
## [1] "/HDF5ArrayAUT000002"
##
## Slot "as_sparse":
## [1] FALSE
##
## Slot "type":
## [1] NA
##
## Slot "dim":
## [1] 64102      8
##
## Slot "chunkdim":
## [1] 64102      8
##
## Slot "first_val":
## [1] 679
```

RleArray and HDF5Array objects

`cbind()` / `rbind()` are delayed:

```
M4 <- cbind(M3, M[1:5, 6:8])
M4

## <5 x 6> matrix of class DelayedMatrix and type "integer":
##      [,1] [,2] [,3] [,4] [,5] [,6]
## [1,] 394  172 2112 1047  770  572
## [2,] 236  168 1867   0    0    0
## [3,] 464  264 5137  799  417  508
## [4,] 175  118 2657  331  233  229
## [5,] 658  241 2735   63   76   60
```

```
seed(M4) # Error! (more than one seed)
```

RleArray and HDF5Array objects

All the operations in the following groups are delayed:

- Arith (+, -, ...)
- Compare (==, <, ...)
- Logic (&, |)
- Math (log, sqrt)
- and more ...

```
M5 <- M == 0
M5

## <64102 x 8> matrix of class DelayedMatrix and type "logical"
##      [,1] [,2] [,3] ... [,7] [,8]
##      [1,] FALSE FALSE FALSE . FALSE FALSE
##      [2,] TRUE TRUE TRUE . TRUE TRUE
##      [3,] FALSE FALSE FALSE . FALSE FALSE
##      [4,] FALSE FALSE FALSE . FALSE FALSE
##      [5,] FALSE FALSE FALSE . FALSE FALSE
##      ... . . . . .
## [64098,] TRUE TRUE TRUE . TRUE TRUE
## [64099,] TRUE TRUE TRUE . TRUE TRUE
## [64100,] TRUE TRUE TRUE . TRUE TRUE
## [64101,] TRUE TRUE TRUE . TRUE TRUE
## [64102,] TRUE TRUE TRUE . TRUE TRUE
```

```
seed(M5)

## An object of class "HDF5ArraySeed"
## Slot "filepath":
## [1] "D:/biocbuild/bbs-3.14-
bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00002.h5"
##
## Slot "name":
## [1] "/HDF5ArrayAUT000002"
##
## Slot "as_sparse":
## [1] FALSE
##
## Slot "type":
## [1] NA
##
## Slot "dim":
## [1] 64102 8
##
## Slot "chunkdim":
## [1] 64102 8
##
## Slot "first_val":
## [1] 679
```

RleArray and HDF5Array objects

```
M6 <- round(M[11:14, ] / M[1:4, ], digits=3)
M6

## <4 x 8> matrix of class DelayedMatrix and type "double":
##      [,1] [,2] [,3] ... [,7] [,8]
## [1,] 0.253 0.375 0.302 . 0.201 0.309
## [2,] Inf   Inf   Inf   .   Inf   Inf
## [3,] 1.122 0.948 1.027 . 1.182 0.935
## [4,] 0.273 0.242 0.802 . 0.575 0.751
```

```
seed(M6) # Error! (more than one seed)
```

Realization

Delayed operations can be **realized** by coercing the DelayedMatrix object to HDF5Array:

```
M6a <- as(M6, "HDF5Array")
M6a

## <4 x 8> matrix of class "HDF5Matrix" and type "double":
##      [,1] [,2] [,3] ... [,7] [,8]
## [1,] 0.253 0.375 0.302 . 0.201 0.309
## [2,] Inf   Inf   Inf   .   Inf   Inf
## [3,] 1.122 0.948 1.027 . 1.182 0.935
## [4,] 0.273 0.242 0.802 . 0.575 0.751
```

```
seed(M6a)

## An object of class "HDF5ArraySeed"
## Slot "filepath":
## [1] "D:/biocbuild/bbs-3.14-
##      bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00003.h5"
##
## Slot "name":
## [1] "/HDF5ArrayAUT000003"
##
## Slot "as_sparse":
## [1] FALSE
##
## Slot "type":
## [1] NA
##
## Slot "dim":
## [1] 4 8
##
## Slot "chunkdim":
## [1] 4 8
##
## Slot "first_val":
## [1] 0.253
```

RleArray and HDF5Array objects

... or by coercing it to RleArray:

```
M6b <- as(M6, "RleArray")
M6b

## <4 x 8> matrix of class RleMatrix and type "double":
##      [,1] [,2] [,3] ... [,7] [,8]
## [1,] 0.253 0.375 0.302 . 0.201 0.309
## [2,] Inf   Inf   Inf   .   Inf   Inf
## [3,] 1.122 0.948 1.027 . 1.182 0.935
## [4,] 0.273 0.242 0.802 . 0.575 0.751
```

```
seed(M6b)

## An object of class "ChunkedRleArraySeed"
## Slot "breakpoints":
## [1] 32
##
## Slot "type":
## [1] "double"
##
## Slot "chunks":
## <environment: 0x000000003725d8c0>
##
## Slot "DIM":
## [1] 4 8
##
## Slot "DIMNAMES":
## [[1]]
## NULL
##
## [[2]]
## NULL
```

Controlling where HDF5 datasets are realized

HDF5 dump management utilities: a set of utilities to control where HDF5 datasets are written to disk.

```
setHDF5DumpFile("~/mydata/M6c.h5")
setHDF5DumpName("M6c")
M6c <- as(M6, "HDF5Array")
```

```
seed(M6c)

## An object of class "HDF5ArraySeed"
## Slot "filepath":
## [1] "C:/Users/biocbuild/Documents/mydata/M6c.h5"
##
## Slot "name":
## [1] "/M6c"
##
## Slot "as_sparse":
## [1] FALSE
##
## Slot "type":
## [1] NA
##
## Slot "dim":
## [1] 4 8
##
## Slot "chunkdim":
## [1] 4 8
##
## Slot "first_val":
## [1] 0.253

h5ls("~/mydata/M6c.h5")

##   group name      otype dclass   dim
## 0      /   M6c H5I_DATASET  FLOAT 4 x 8
```

showHDF5DumpLog()

```
showHDF5DumpLog()
```

```
## [2021-09-23 20:35:07] #1 In file 'D:/biocbuild/bbs-3.14-bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00001.h5': creation of dataset  
'/HDF5ArrayAUTO000001' (64102x8:integer, chunkdims=64102x8, level=6)  
## [2021-09-23 20:35:07] #2 In file 'D:/biocbuild/bbs-3.14-bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00002.h5': creation of dataset  
'/HDF5ArrayAUTO000002' (64102x8:integer, chunkdims=64102x8, level=6)  
## [2021-09-23 20:35:07] #3 In file 'D:/biocbuild/bbs-3.14-bioc/tmpdir/RtmpoJNt1M/HDF5Array_dump/auto00003.h5': creation of dataset  
'/HDF5ArrayAUTO000003' (4x8:double, chunkdims=4x8, level=6)  
## [2021-09-23 20:35:08] #4 In file 'C:/Users/biocbuild/Documents/mydata/M6c.h5': creation of dataset 'M6c' (4x8:double,  
chunkdims=4x8, level=6)
```

Block processing

The following operations are NOT delayed. They are implemented via a *block processing* mechanism that loads and processes one block at a time:

- operations in the Summary group (max, min, sum, any, all)
- mean
- Matrix row/col summarization operations (col/rowSums, col/rowMeans, ...)
- anyNA, which
- apply
- and more ...

RleArray and HDF5Array objects

```
DelayedArray::set_verbose_block_processing(TRUE)

## [1] FALSE

colSums(M)

## Processing block [[1/1, 1/1]] ... OK

## [1] 20637971 18809481 25348649 15163415 24448408 30818215 19126151 21164133
```

Control the block size:

```
getAutoBlockSize()

## [1] 1e+08

setAutoBlockSize(1e6)

## automatic block size set to 1e+06 bytes (was 1e+08)

colSums(M)

## Processing block [[1/1, 1/1]] ...
## OK

## [1] 20637971 18809481 25348649 15163415 24448408 30818215 19126151 21164133
```

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1. Load the "airway" dataset.
2. It's wrapped in a SummarizedExperiment object. Get the count data as an ordinary matrix.
3. Wrap it in an HDF5Matrix object: (1) using `writeHDF5Array()`; then (2) using coercion.
4. When using coercion, where has the data been written on disk?
5. See `?setHDF5DumpFile` for how to control the location of "automatic" HDF5 datasets. Try to control the destination of the data when coercing.

6. Use `showHDF5DumpLog()` to see all the HDF5 datasets written to disk during the current session.
7. Try some operations on the `HDF5Matrix` object: (1) some delayed ones; (2) some non-delayed ones (block processing).
8. Use `DelayedArray::set_verbose_block_processing(TRUE)` to see block processing in action.
9. Control the block size with `setAutoBlockSize()`.

10. Stick the `HDF5Matrix` object back in the `SummarizedExperiment` object. The resulting object is an "HDF5-backed `SummarizedExperiment` object".

11. The HDF5-backed `SummarizedExperiment` object can be manipulated (almost) like an in-memory `SummarizedExperiment` object. Try `[`, `cbind`, `rbind` on it.

12. The *SummarizedExperiment* package provides `saveHDF5SummarizedExperiment` to save a `SummarizedExperiment` object (HDF5-backed or not) as an HDF5-backed `SummarizedExperiment` object. Try it.

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Block processing improvements

Block genometry: (1) better by default, (2) let the user have more control on it

Support multicore

Expose it: `blockApply()`

HDF5Array improvements

Store the `dimnames` in the HDF5 file (in *HDF5 Dimension Scale datasets* - <https://www.hdfgroup.org/HDF5/Tutor/h5dimscale.html>)

Use better automatic chunk geometry when realizing an HDF5Array object

Block processing should take advantage of the chunk geometry (e.g. `realize()` should use blocks that are clusters of chunks)

Unfortunately: not possible to support multicore realization at the moment (HDF5 does not support concurrent writing to a dataset yet)

RleArray improvements

Let the user have more control on the chunk geometry when constructing/realizing an RleArray object

Like for HDF5Array objects, block processing should take advantage of the chunk geometry

Support multicore realization

Provide C/C++ low-level API for direct row/column access from C/C++ code (e.g. from the *beachmat* package)