An Introduction to the BigMatrix Package

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1 Introduction

This package defines a "BigMatrix" ReferenceClass which adds safety and convenience features to the file-backed.big.matrix class from the bigmemory package. BigMatrix protects against segfaults by monitoring and gracefully restoring the connection to on-disk data and it also protects against accidental data modification with a filesystem-based permissions system. We provide utilities for using BigMatrix-derived classes as assayData matrices within the Biobase package's eSet family of classes. BigMatrix provides some optimizations related to attaching to, and indexing into, file-backed matrices with dimnames. Additionally, the package provides a "BigMatrixFactor" class, a file-backed matrix with factor properties.

```
> library(BigMatrix)
> data.file = file.path(tempdir(),"bigmat","ds")
> x = matrix(1:9,ncol=3,dimnames=list(letters[1:3],LETTERS[1:3]))
> ds = BigMatrix(x,data.file)
> ds[,1] = 3:1
> ds[,1]
```

```
a b c
3 2 1
```

2 Re-attaching to on-disk data as necessary

When a big.matrix object is attached to it's on-disk data, an external pointer is used to connect the R object to a C++ data structure. When a big.matrix object is not attached, like when it is loaded from an RData file, this pointer is nil. Any access to this nil pointer will crash R. The BigMatrix package provides a BigMatrix class that prevents such a crash by controlling access to the external pointer. Additionally, BigMatrix objects remember the location of their on-disk components and automatically re-attach themselves as necessary.

This kind of thing would be helpful if you, for example, chose to save your new BigMatrix object to disk for later use. You might save your object using R's built in save or saveRDS functions.

```
> ds$descpath
```

```
[1] "/tmp/RtmpHvIOm9/bigmat/ds.desc.rds"
```

```
> saveRDS(ds,file=file.path(tempdir(),"foo.rds"))
> new.ds = readRDS(file=file.path(tempdir(),"foo.rds"))
> new.ds[1:2,2:3]
```

```
Attaching to on-disk data: /tmp/RtmpHvIOm9/bigmat/ds.desc.rds ...
  B C
a 4 7
b 5 8
```

3 Files

The bigmemory package creates two files for each object, and BigMatrix adds a third. The bigmemory package creates one binary file for the matrix data (the "backingfile") and one text file with meta-data about its matrix (the "descriptor" file). The functions dget and dput are used to access this meta-data. For large matrices with dimnames, this can take a while. BigMatrix uses readRDS and saveRDS to store meta-data in a third file, which requires about 1/10 the time to read when it's time to attach an object to the backingfile. Use of a separate file allows access to the on-disk data via big.matrix or BigMatrix objects.

4 Limiting Write Permissions

BigMatrix provides OS-level write permissions to the on-disk data. With both big.matrix and BigMatrix, a user must always have read and write permissions to the backingfile. BigMatrix uses the file system permissions on the meta-data file, checking for write permission before allowing the user to alter any of the on-disk data. This allows for a measure of safety when BigMatrix data are used as a group resource.

```
> ds[1,1] = 5
> Sys.chmod(ds$descpath,"0444")
> tryCatch( { ds[1,1] = 10 }, error = function(e) { print(e) } )

<simpleError in x$setValues(i, j, value): You do not have write permission on the 'desc' file for this Bi

> Sys.chmod(ds$descpath,"0644")
> ds[1,1] = 10
> ds[,]

   A B C
a 10 4 7
b  2 5 8
c  1 6 9

> as(ds,"matrix")

   A B C
a 10 4 7
b  2 5 8
c  1 6 9
```

5 S4 Style Access

The BigMatrix class uses R's Reference Class system. Any change to the matrix portion of the data has on-disk side effects, so it seems natural that any other changes to the object should have the same behavior. In order to give BigMatrix the same API as a base matrix or big.matrix class, certain S4-style methods are provided. ReferenceClass objects are relatively new to R and unfamiliar to many users, so you may want to review the ReferenceClasses help page.

```
> nrow(ds)

[1] 3

> ds$nrow()

[1] 3
```

```
> ncol(ds)

[1] 3

> ds$ncol()

[1] 3

> dim(ds)

[1] 3 3

> ds$dim()

[1] 3 3

> dimnames(ds)

[[1]]
[1] "a" "b" "c"

[[2]]
[1] "A" "B" "C"

> ds$dimnames()

[[1]]
[1] "a" "b" "c"

[[2]]
[1] "A" "B" "C"

> length(ds)

[1] 9

> ds$length()

[1] 9
```

6 BigMatrixFactor

The BigMatrix package adds a "BigMatrixFactor" class to provide a means to store large matrices of characters. On the file system, these are stored as the C type char or int (8 or 32 bits), depending on the number of levels in the factor. Subsetting a BigMatrixFactor returns a base matrix that is also a factor. This provides a convenient way to convert between integer and character representations of the data.

```
> data.file = file.path(tempdir(),"bigmat","fs")
> x = matrix( c(rep(1,5),rep(2,4)) ,ncol=3,dimnames=list(letters[1:3],LETTERS[1:3]))
> fs = BigMatrixFactor(x,data.file,levels=c("AA","BB"))
> fs[,]

  A  B  C
a AA AA BB
b AA AA BB
c AA BB BB
Levels: AA BB
```

```
> as(fs,"factor")

  A  B  C
a AA AA BB
b AA AA BB
c AA BB BB
Levels: AA BB

> as(fs,"matrix")

  A B C
a 1 1 2
b 1 1 2
c 1 2 2

> fs$levels

[1] "AA" "BB"

> levels(fs)

[1] "AA" "BB"
```

However, you may want to set the S3 class of this matrix/factor to 'matrix' in some cases, like when you need to maintain its shape.

```
> x = as(fs,"factor")
> x

  A  B  C
a AA AA BB
b AA AA BB
c AA BB BB
Levels: AA BB

> x == "BB"

[1] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE

> y = as(fs,"matrix")
> y

  A B C
a 1 1 2
b 1 1 2
c 1 2 2

> y == 2

      A     B    C
a FALSE FALSE TRUE
b FALSE FALSE TRUE
c FALSE  TRUE TRUE

> rowMeans( y == 2 )

        a         b         c
0.3333333 0.3333333 0.6666667
```

7 Use with Biobase and eSet-derived Classes

Either class can be used as an assayDataElement in the assayData slot of the familiar BioConductor eSet-derived classes. We provide utility functions to deal with relocated BigMatrix files and to attach all of an eSet's BigMatrix assayDataElements. Of course, you can also just let them attach themselves as necessary.

```
> library(Biobase)
> eset = ExpressionSet()
> assayDataElement(eset,"exprs") = ds
> exprs(eset)[1:2,2:3]

  B C
a 4 7
b 5 8

> new.dir = file.path(tempdir(),"newbigmat")
> dir.create(new.dir,showWarnings=FALSE)
> file.copy(ds$descpath, new.dir)

[1] TRUE

> file.copy(ds$datapath, new.dir)

[1] TRUE

> updateAssayDataElementPaths( assayData(eset), new.dir )
> assayDataElement(eset,"exprs")$descpath

[1] "/tmp/RtmpHvI0m9/newbigmat/ds.desc.rds"

> attachAssayDataElements( eset )
>
```

8 Optimal Usage

Using dimension names can slow down access to a BigMatrix/big.matrix object considerably. Indexing into a big.matrix by dimname is considerably slower indexing by integer. BigMatrix has an optimization to reduce this penalty.

Reading from a BigMatrix/big.matrix with dimnames is also slower, as transferring dimnames from big.matrix's C++ representation to R and adding them to the numeric data from the matrix takes some time. Typically, this takes much more time than just reading the numeric data.

Future optimizations may remove these penalties without changing the API, but when speed is critical, you will want to avoid indexing by character values and you may want to avoid having dimnames altogether.