# BufferedMatrix: Introduction

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### 1 Introduction

This document is intended to introduce the BufferedMatrix package and how it may be used. It is very important to know that this package provides infrastructure rather than an analysis methods as most other BioConductor packages do. It is not intended to be used directly by end-users. Instead it is aimed at developers of other packages. The main purpose of this package is to provide the BufferedMatrix object. This document will explain how to use the BufferedMatrix object at the R level. There is also a C language interface to dealing with BufferedMatrix objects, but that will not be discussed here.

#### 2 What is a BufferedMatrix?

A BufferedMatrix object stores numerical data in a tabular format, with most of the data primarily stored outside main memory on the file system. Figure 1 shows that a BufferedMatrix consists of data values arranged in rows and columns. The BufferedMatrix object implemented in this package is optimized for situations where the number of rows in much larger than the number of columns. The word Buffered is used because frequently used parts of the BufferedMatrix may be kept in main memory for increased speed. It is intended that users of the BufferedMatrix will be unaware of what is and is not in memory. Note that although the word Matrix is part of the name of the object it does not imply that you may treat a BufferedMatrix object exactly like a Matrix in all situations. For instance BufferedMatrix objects are passed by reference rather than by value, are not designed for using with Matrix algebra and can not automatically be passed to all pre-existing functions that expect ordinary matrices (particularly functions that use C code). More details about these issues will be discussed a little later in this document.

But first it is time to explore how to use the package. As with other packages we use library to load the package.

#### > library(BufferedMatrix)

To create a BufferedMatrix we use the createBufferedMatrix function. This function takes up to six arguments, but only the first one must be provided. To start with use:

#### > X <- createBufferedMatrix(10000)</pre>

to create a BufferedMatrix with 10000 rows and 0 columns. Notice how only the number of rows must be supplied when creating a *BufferedMatrix*. This is because BufferedMatrix objects fix the number of Rows they store, but allow you to dynamically add columns when needed. It is not possible however to remove columns from a BufferedMatrix. Just like all R objects typing the name of the object will show you some basic information (or the contents) of the object. In this case

#### > X

BufferedMatrix object Matrix size: 10000 0 Buffer size: 1 1

Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes

Prefix: BM Mode: Col mode Read Only: FALSE

Memory usage: 161 bytes. Disk usage: 0 bytes.

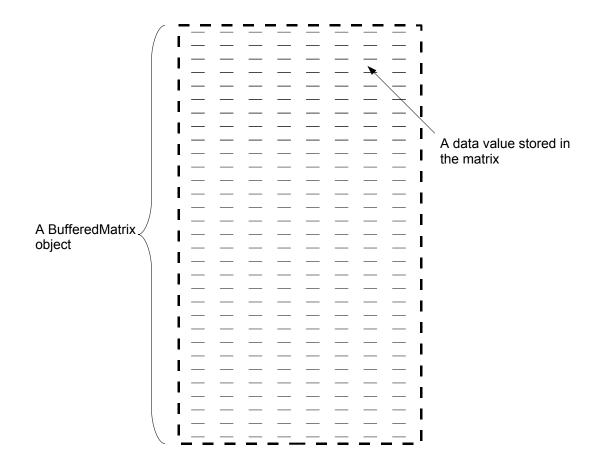


Figure 1: A BufferedMatrix stores data values in tabular format. In the figures the dashed lines means that the data is stored outside main memory on the filesystem

Notice that basic summary information about the matrix is displayed in this case. We will discuss what this information means a little later. We could use the AddColumn function to add columns to our matrix like this

#### > AddColumn(X)

BufferedMatrix object Matrix size: 10000 1 Buffer size: 1 1

Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes

Prefix: BM Mode: Col mode Read Only: FALSE

Memory usage: 78.4 Kilobytes. Disk usage: 78.1 Kilobytes.

#### > AddColumn(X)

BufferedMatrix object Matrix size: 10000 2 Buffer size: 1 1

Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes

Prefix: BM Mode: Col mode Read Only: FALSE

Memory usage: 78.5 Kilobytes. Disk usage: 156.2 Kilobytes.

#### > X

BufferedMatrix object Matrix size: 10000 2 Buffer size: 1 1

Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes

Prefix: BM Mode: Col mode Read Only: FALSE

Memory usage: 78.5 Kilobytes. Disk usage: 156.2 Kilobytes.

Of course it might have been more convinent just to instantiate our BufferedMatrix object from the beginning as having 10000 rows and 2 columns. This would be acomplished using

#### > X <- createBufferedMatrix(10000,2)</pre>

Of course BufferedMatrix objects use buffers to temporarily store some of its contents in main memory, rather than on the filesystem. There are two types of buffering provided by BufferedMatrix objects. This are ColMode and RowMode. The default mode when you create a BufferedMatrix is to be in ColMode. Figure 2 demonstrates the situation in ColMode. Specifically, the entire contents of a given number of columns are stored completely in RAM, with the rest of the data remaining on the file system. There is no requirement that these columns be contiguous. When most of your operations are to be done in a column-wise manner it is more efficient to be in ColMode.

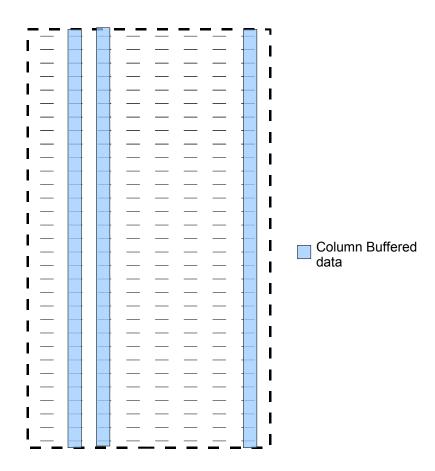


Figure 2: Column Buffers hold selected columns in RAM. This speeds up access to data. Column Buffers are always active

The other main buffering mode is RowMode. Figure 3 illustrates the situation when in RowMode. Note that when in row mode a block of contiguous rows across all columns of the BufferedMatrix is kept in main memory. RowMode is designed for situations where you need to access a fixed set of closely spaced rows of the matrix. Note that RowMode

is considered a secondary buffering mode and that the column buffers are also present when in this mode.

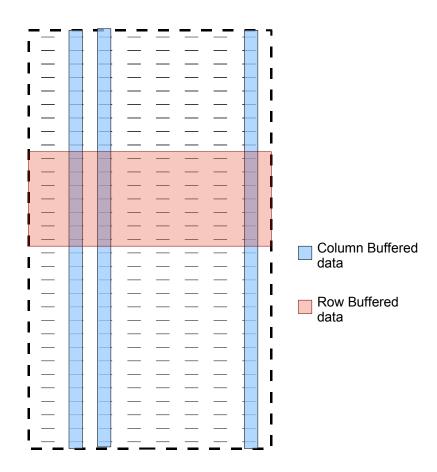


Figure 3: Row Buffers hold a selected contiguous block of rows in RAM. Row Buffers exist only when the BufferedMatrix is in RowMode.

As previously mentioned before, all *BufferedMatrix* objects start in ColMode. To switch to RowMode you can use the RowMode function like this:

#### > RowMode(X)

<pointer: 0x5ae643f3f8f0>

To switch back to ColMode use

> ColMode(X)

<pointer: 0x5ae643f3f8f0>

When you create the BufferedMatrix you can control the size of these Buffers in terms of number of columns or number of rows. In particular, suppose we wanted a 10000 by 5 matrix with 1 column buffered and 500 rows buffered when in row mode, this could be done by

```
> X <- createBufferedMatrix(10000,5,bufferrows=500,buffercols=1)
```

You can also use set.buffer.dim function to set or change these after the matrix has been create. For instance to change it to 2 columns buffered and 100 rows use:

```
> set.buffer.dim(X,100,2)
```

<pointer: 0x5ae643be92a0>

There are two additional arguments to createBufferedMatrix. The first is prefix which is a string that will be used to start each temporary file name used for the filesystem storage of the *BufferedMatrix*, by default this is "BM". The second is directory which specifies where these temporary files are to be stored. By default this directory is the current working directory.

There are several functions to get this, and additional, information about an already created BufferedMatrix.

```
> memory.usage(X)
```

[1] 160619

> disk.usage(X)

[1] 4e+05

> nrow(X)

[1] 10000

> ncol(X)

[1] 5

> dim(X)

[1] 10000 5

> buffer.dim(X)

[1] 100 2

```
> prefix(X)
[1] "BM"
> directory(X)
[1] "/tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes"
> is.RowMode(X)
[1] FALSE
> is.ColMode(X)
```

There is one other important mode that you may switch a *BufferedMatrix* in and out of. This is *ReadOnly* mode. What this means is that you can access data values stored in the matrix but you can not change them. This provides speed-up in some situations because the current buffer does not need to be flushed out to the filesystem when an attempt is made to access a value currently not stored in the buffer. The

function ReadOnlyMode is used to toggle between the two states.

```
> ReadOnlyMode(X)
<pointer: 0x5ae643be92a0>
> is.ReadOnlyMode(X)
[1] TRUE
> ReadOnlyMode(X)
<pointer: 0x5ae643be92a0>
> is.ReadOnlyMode(X)
```

[1] TRUE

[1] FALSE

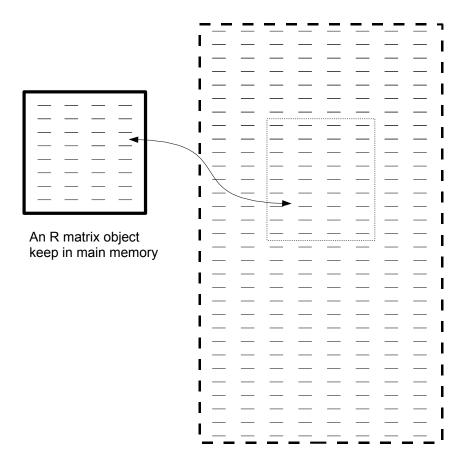


Figure 4: Subsetting operators pull data out of the Buffered Matrix object and into R matrix objects or vice versa.

# 3 Accessing and Manipulating data stored within a BufferedMatrix

Data is accessed from *BufferedMatrix* objects using similar indexing procedures to those you would use with a standard *matrix* object. In particular you can use the [ aind [<- operators to see or replace data in an Buffered Matrix. Figure 4 demonstrates how indexing and assignment operations are set up to occur with *BufferedMatrix* objects. Specifically, when you index part of the BufferedMatrix an ordinary R matrix is created and the data requested copied from the BufferedMatrix. This matrix is then no longer linked to the data in the BufferedMatrix.

For example

```
> X <- createBufferedMatrix(20,2)</pre>
> X[1:20,] <- 1:40
> B <- X[1:5,]
> B
      [,1] [,2]
[1,]
         1
              21
[2,]
         2
              22
[3,]
         3
              23
[4,]
         4
              24
[5,]
         5
              25
> B[1:2,] <- B[1:2,]^2
> B
      [,1] [,2]
[1,]
            441
         1
[2,]
         4
            484
[3,]
         3
              23
[4,]
         4
              24
[5,]
         5
              25
> X[1:5,]
      [,1] [,2]
[1,]
              21
[2,]
         2
              22
[3,]
         3
              23
[4,]
         4
              24
[5,]
         5
              25
```

Similarly, assignments using the indexing operators copy the data from the R matrix or vector into the specified location of the BufferedMatrix.

```
> X[1:5,] <- B
> X[1:5,]
     [,1] [,2]
[1,]
         1
            441
[2,]
         4
            484
[3,]
         3
             23
[4,]
         4
             24
[5,]
         5
             25
```

As with ordinary R  $\it matrix$  objects we may have column or row name indices. For example:

> rownames(X)

NULL

> colnames(X)

NULL

```
> rownames(X) <- letters[1:20]
> colnames(X) <- month.abb[1:2]</pre>
```

and these can be used interchangably with numerical indexing values.

Jan

a 1

b 4

BufferedMatrix objects also support logical indexing. eg

> X[rep(c(TRUE,FALSE),10),1]

Jan

- a 1
- c 3
- e 5
- g 7

i 9 k 11 m 13 o 15 q 17 s 19

Sometimes it might be useful to create another *BufferedMatrix* out of an existing one. For this purpose the subBufferedMatrix command may be used. This function operates in a similar manner to indexing operators, but instead of copying the data into an R matrix another BufferedMatrix is produced. Figure 5 illustrates this procedure.

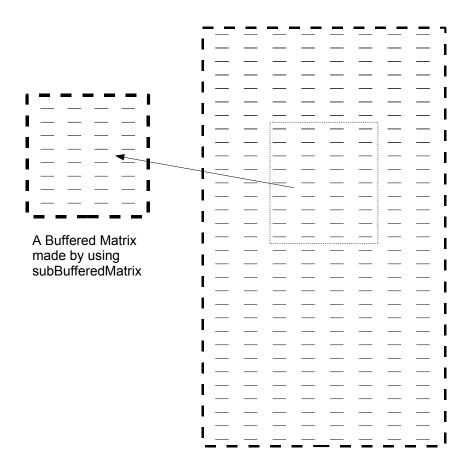


Figure 5: Using subBufferedMatrix creates a new BufferedMatrix containing a subset of the data stored in the BufferedMatrix

> Y <- subBufferedMatrix(X,1:5,1:2)
> Y

BufferedMatrix object

Matrix size: 5 2 Buffer size: 1 1

Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes

Prefix: BM Mode: Col mode Read Only: FALSE

Memory usage: 387 bytes. Disk usage: 80 bytes.

## 4 Functions for summarizing a BufferedMatrix

Sometimes it is useful to generate summary statistic values from a *BufferedMatrix* object. While it would be possible to do this by writing your own code using loops and indexing a number of more optimized functions have been provided for this purpose. These functions concentrate on getting the maximum, minimum, means, variances and so forth. The try to minimize buffer misses as much as possible.

```
> X <- createBufferedMatrix(10,3)</pre>
```

- > X[1:10,] <- (1:30)^2
- > Max(X)
- [1] 900
- > Min(X)
- [1] 1
- > mean(X)
- [1] 315.1667
- > Sum(X)
- [1] 9455
- > Var(X)
- [1] 79106.83
- > Sd(X)
- [1] 281.2594

It may also be useful to get these values for each column or each row.

- > rowMeans(X)
  - [1] 187.6667 210.6667 235.6667 262.6667 291.6667 322.6667 355.6667 390.6667
  - [9] 427.6667 466.6667
- > colMeans(X)
- [1] 38.5 248.5 658.5
- > rowSums(X)
- [1] 563 632 707 788 875 968 1067 1172 1283 1400
- > colSums(X)
- [1] 385 2485 6585
- > rowVars(X)
  - [1] 51733.33 60933.33 70933.33 81733.33 93333.33 105733.33 118933.33
  - [8] 132933.33 147733.33 163333.33
- > colVars(X)
- [1] 1167.833 8867.833 23901.167
- > rowSd(X)
  - [1] 227.4496 246.8468 266.3331 285.8904 305.5050 325.1666 344.8671 364.6002
  - [9] 384.3609 404.1452
- > colSd(X)
- [1] 34.17358 94.16917 154.60002
- > rowMax(X)
- [1] 441 484 529 576 625 676 729 784 841 900
- > colMax(X)
- [1] 100 400 900
- > rowMin(X)
- [1] 1 4 9 16 25 36 49 64 81 100
- > colMin(X)
- [1] 1 121 441

# 5 Applying your own function to the rows or columns of a BufferedMatrix

While many useful functions are provided for carrying out row-wise or column-wise operations, you may want to use your own function to do a different summarization. This may be done using the rowApply and colApply functions. For example suppose you wanted to write a function which computed the sum of the cube roots of the elements of a column. This would be done like this:

Note that if your *BufferedMatrix* is large and you are not in RowMode, with a sufficiently sized row buffer, then calls to rowApply will be very slow.

It is also possible to use a function which returns more than one item. In this case, rather than returning a vector another BufferedMatrix will be returned.

```
> Y <- colApply(X,sort,decreasing=TRUE)
> is(Y,"BufferedMatrix")
```

#### [1] TRUE

Note that colApply and rowApply assume that your function returns a fixed length vector.

# 6 Elementwise transformation of BufferedMatrix objects

In some situations it might be useful to transform each element of your *BufferedMatrix*. For instance log or exponential transformations, square roots or arbitrary powers. Unlike when you ordinarily apply these functions to an R matrix, when you apply these function to *BufferedMatrix* objects, the object is not copied before being transformed. In otherwords these functions do not leave the *BuffferedMatrix* untouched.

```
> exp(X)
<pointer: 0x5ae643858c30>
> log(X)
<pointer: 0x5ae643858c30>
> sqrt(X)
<pointer: 0x5ae643858c30>
> pow(X,2.0)
```

If you have a customized function that you want to apply in an element-wise fashion you can use the ewApply function. Note that the function you supply must return only a single value when it is given an argument of length 1 and must return a vector of length n if given a vector of length n. It is best that you design your input function to operate in a vectorized manner.

```
> my.function <- function(x){
+    x^2 +3*abs(x) - 9
+ }
> ewApply(X, my.function)

BufferedMatrix object
Matrix size: 10 3
Buffer size: 1 1
Directory: /tmp/RtmpIWTeqx/Rbuild10b4cc348dedea/BufferedMatrix/vignettes
Prefix: BM
Mode: Col mode
Read Only: FALSE
Memory usage: 513 bytes.
Disk usage: 240 bytes.
```

# 7 Converting between BufferedMatrix and Matrix objects

It is possible to convert a *BufferedMatrix* into a *matrix* and vice versa. But in most cases you will not want to do this because your *BufferedMatrix* may be too large to keep completely in the RAM available to R.

To convert a BufferedMatrix to a Matrix use:

```
> Z <- as(X,"matrix")
> class(Z)

[1] "matrix" "array"

   To make a Matrix become a BufferedMatrix use:
> A <- as(Z,"BufferedMatrix")
> class(A)

[1] "BufferedMatrix"
attr(,"package")
[1] "BufferedMatrix"
```

### 8 BufferedMatrix objects are pass-by reference

As previously mentioned when you pass an *BufferedMatrix* to a function you are passing it by reference. This means that if the function operates on the *BufferedMatrix* using a function that can change values stored within the *BufferedMatrix* then it is changed in the calling environment. This differs from the behaviour of a normal R matrix.

```
> X <- createBufferedMatrix(50,10)</pre>
> X[1:50,] <- 1:500
> Y <- as(X,"matrix")</pre>
> my.function <- function(a.matrix){</pre>
    a.matrix[,1:10] <- a.matrix[,sample(1:10,10)]
+ }
> X[1:5,]
     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]
                            201
                                  251
             51
                 101
                       151
                                        301
                                             351
                                                   401
                                                         451
[2,]
                 102
                       152
                            202
                                  252
                                        302
                                             352
                                                   402
                                                          452
[3,]
                 103
                       153
                            203
                                  253
                                        303
                                             353
                                                   403
        3
             53
                                                         453
[4,]
        4
             54
                 104
                       154
                            204
                                  254
                                        304
                                             354
                                                   404
                                                          454
[5,]
        5
             55
                 105
                       155
                            205
                                  255
                                        305
                                             355
                                                   405
                                                         455
```

```
> my.function(X)
> X[1:5,]
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]
      201
              51
                  401
                        451
                              251
                                    151
                                            1
                                                351
                                                      101
                                                             301
[2,]
                                            2
      202
              52
                  402
                        452
                              252
                                    152
                                                352
                                                      102
                                                             302
[3,]
      203
              53
                  403
                        453
                              253
                                    153
                                            3
                                                353
                                                      103
                                                             303
[4,]
      204
                  404
                        454
                              254
                                            4
                                                354
                                                      104
              54
                                    154
                                                             304
[5,]
                        455
                              255
                                            5
      205
              55
                  405
                                    155
                                                355
                                                      105
                                                             305
> Y[1:5,]
      [,1]
           [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]
         1
              51
                  101
                        151
                              201
                                    251
                                          301
                                                351
                                                      401
                                                             451
[2,]
         2
              52
                  102
                        152
                              202
                                    252
                                          302
                                                352
                                                      402
                                                             452
[3,]
                  103
                        153
                              203
                                    253
                                          303
                                                353
                                                      403
         3
              53
                                                             453
[4,]
         4
                  104
                        154
                              204
                                    254
                                          304
                                                354
              54
                                                      404
                                                             454
[5,]
         5
              55
                  105
                        155
                              205
                                    255
                                          305
                                                355
                                                      405
                                                             455
> my.function(Y)
> Y[1:5,]
           [,2]
                 [,3] [,4] [,5] [,6] [,7]
                                               [,8]
                                                     [,9] [,10]
[1,]
         1
              51
                  101
                        151
                              201
                                    251
                                          301
                                                351
                                                      401
                                                             451
[2,]
         2
              52
                        152
                              202
                                    252
                                                352
                                                      402
                  102
                                          302
                                                             452
[3,]
         3
              53
                  103
                        153
                              203
                                    253
                                          303
                                                353
                                                      403
                                                             453
[4,]
         4
              54
                  104
                        154
                              204
                                    254
                                          304
                                                354
                                                      404
                                                             454
[5,]
         5
              55
                  105
                        155
                              205
                                    255
                                          305
                                                355
                                                      405
                                                             455
```

There is one exception to the pass-by reference rule, column and row names are passed by value, meaning that modifications to dimension names within a calling function have no effect on the dimension names in the calling environment. However, this may be changed in future releases so you should not rely on this behaviour.

In situations where you want to simulate call by value you can use the duplicate function. This will make a copy of the *BufferedMatrix*.

```
> X <- createBufferedMatrix(50,10)
> X[1:50,] <- 1:500
> my.function <- function(my.bufmat){
+ internal.bufmat <- duplicate(my.bufmat)
+ internal.bufmat[,1:10] <- internal.bufmat[,sample(1:10,10)]
+ }
> X[1:5,]
```

```
[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]
         1
             51
                        151
                              201
                                    251
                                          301
                                               351
                                                     401
                  101
                                                            451
[2,]
         2
              52
                  102
                        152
                              202
                                    252
                                          302
                                               352
                                                     402
                                                            452
[3,]
         3
             53
                  103
                        153
                              203
                                    253
                                          303
                                               353
                                                     403
                                                            453
[4,]
         4
             54
                  104
                        154
                              204
                                    254
                                          304
                                               354
                                                     404
                                                            454
[5,]
         5
             55
                  105
                        155
                              205
                                    255
                                          305
                                               355
                                                     405
                                                            455
```

> my.function(X)

> X[1:5,]

```
[,2]
                 [,3] [,4] [,5] [,6] [,7]
                                               [,8]
                                                     [,9] [,10]
[1,]
         1
              51
                  101
                              201
                                    251
                                          301
                                                351
                                                      401
                        151
                                                             451
[2,]
         2
              52
                              202
                                    252
                                                      402
                  102
                        152
                                          302
                                                352
                                                             452
[3,]
         3
              53
                  103
                        153
                              203
                                    253
                                          303
                                                353
                                                      403
                                                             453
[4,]
         4
              54
                  104
                        154
                              204
                                    254
                                          304
                                                354
                                                      404
                                                             454
         5
[5,]
                  105
                              205
                                    255
              55
                        155
                                          305
                                                355
                                                      405
                                                             455
```

Table 1 summarizes which functions modify and those don't modify BufferedMatrix objects.

### 9 Future Enhancements

Currently *BufferedMatrix* objects can not properly serialized. That means you can not save and reload a BufferedMatrix between R sessions. This is an issue to be addressed in a future release of the BufferedMatrix package.

| Functions that do not  | Functions that do      |
|------------------------|------------------------|
| modify data stored in  | modify data stored in  |
| BufferedMatrix objects | BufferedMatrix objects |
| [                      | [<-                    |
| Max                    | exp                    |
| Min                    | log                    |
| mean                   | sqrt                   |
| Sum                    | pow                    |
| Var                    | ewApply                |
| Sd                     | RowMode                |
| rowMeans               | ColMode                |
| colMeans               | ReadOnlyMode           |
| rowSums                | AddColumn              |
| colSums                |                        |
| rowVars                |                        |
| colVars                |                        |
| rowSd                  |                        |
| colSd                  |                        |
| rowMax                 |                        |
| colMax                 |                        |
| rowMin                 |                        |
| colMin                 |                        |
| colApply               |                        |
| rowApply               |                        |
| duplicate              |                        |
| as                     |                        |
| ncol                   |                        |
| nrow                   |                        |
| is.ColMode             |                        |
| is.RowMode             |                        |
| set.buffer.dim         |                        |
| prefix                 |                        |
| directory              |                        |
| filenames              |                        |
| subBufferedMatrix      |                        |
| is.ReadOnlyMode        |                        |
| memory.usage           |                        |
| disk.usage             |                        |

Table 1: A breakdown of functions that do and do not modify data stored in or how it is stored in BufferedMatrix objects.