

The *Biostrings* 2 classes (work in progress)

Hervé Pagès

December 8, 2024

Contents

| | | |
|----------|---|----------|
| 1 | Introduction | 1 |
| 2 | The <i>XString</i> class and its subsetting operator <code>[]</code> | 2 |
| 3 | The <code>==</code> binary operator for <i>XString</i> objects | 3 |
| 4 | The <i>XStringViews</i> class and its subsetting operators <code>[]</code> and <code>[]</code> | 4 |
| 5 | A few more <i>XStringViews</i> objects | 5 |
| 6 | The <code>==</code> binary operator for <i>XStringViews</i> objects | 6 |
| 7 | The <code>start</code>, <code>end</code> and <code>width</code> methods | 6 |

1 Introduction

This document briefly presents the new set of classes implemented in the *Biostrings* 2 package. Like the *Biostrings* 1 classes (found in *Biostrings* v 1.4.x), they were designed to make manipulation of big strings (like DNA or RNA sequences) easy and fast. This is achieved by keeping the 3 following ideas from the *Biostrings* 1 package: (1) use R external pointers to store the string data, (2) use bit patterns to encode the string data, (3) provide the user with a convenient class of objects where each instance can store a set of views *on the same* big string (these views being typically the matches returned by a search algorithm).

However, there is a flaw in the *BioString* class design that prevents the search algorithms to return correct information about the matches (i.e. the views) that they found. The new classes address this issue by replacing the *BioString* class (implemented in *Biostrings* 1) by 2 new classes: (1) the *XString* class used to represent a *single* string, and (2) the *XStringViews* class used to represent a set of views *on the same XString* object, and by introducing new implementations and new interfaces for these 2 classes.

2 The *XString* class and its subsetting operator [

The *XString* is in fact a virtual class and therefore cannot be instantiated. Only subclasses (or subtypes) *BString*, *DNAString*, *RNAString* and *AAString* can. These classes are direct extensions of the *XString* class (no additional slot).

A first *BString* object:

```
> library(Biostrings)
> b <- BString("I am a BString object")
> b
```

```
21-letter BString object
seq: I am a BString object
```

```
> length(b)
```

```
[1] 21
```

A *DNAString* object:

```
> d <- DNAString("TTGAAAA-CTC-N")
> d
```

```
13-letter DNAString object
seq: TTGAAAA-CTC-N
```

```
> length(d)
```

```
[1] 13
```

The differences with a *BString* object are: (1) only letters from the *IUPAC extended genetic alphabet* + the gap letter (-) are allowed and (2) each letter in the argument passed to the *DNAString* function is encoded in a special way before it's stored in the *DNAString* object.

Access to the individual letters:

```
> d[3]
```

```
1-letter DNAString object
seq: G
```

```
> d[7:12]
```

```
6-letter DNAString object
seq: A-CTC-
```

```
> d[]
```

```
13-letter DNAString object
seq: TTGAAAA-CTC-N
```

```
> b[length(b):1]
```

```
21-letter BString object  
seq: tcejbo gnirtSB a ma I
```

Only *in bounds* positive numeric subscripts are supported.

In fact the subsetting operator for *XString* objects is not efficient and one should always use the `subseq` method to extract a substring from a big string:

```
> bb <- subseq(b, 3, 6)  
> dd1 <- subseq(d, end=7)  
> dd2 <- subseq(d, start=8)
```

To *dump* an *XString* object as a character vector (of length 1), use the `toString` method:

```
> toString(dd2)
```

```
[1] "-CTC-N"
```

Note that `length(dd2)` is equivalent to `nchar(toString(dd2))` but the latter would be very inefficient on a big *DNAStrng* object.

[TODO: Make a generic of the `substr()` function to work with *XString* objects. It will be essentially doing `toString(subseq())`.]

3 The == binary operator for *XString* objects

The 2 following comparisons are TRUE:

```
> bb == "am a"  
> dd2 != DNAStrng("TG")
```

When the 2 sides of `==` don't belong to the same class then the side belonging to the “lowest” class is first converted to an object belonging to the class of the other side (the “highest” class). The class (pseudo-)order is *character* < *BString* < *DNAStrng*. When both sides are *XString* objects of the same subtype (e.g. both are *DNAStrng* objects) then the comparison is very fast because it only has to call the C standard function `memcmp()` and no memory allocation or string encoding/decoding is required.

The 2 following expressions provoke an error because the right member can't be “upgraded” (converted) to an object of the same class than the left member:

```
> bb == ""  
  
> d == bb
```

When comparing an *RNAString* object with a *DNAStrng* object, U and T are considered equals:

```
> r <- RNAString(d)  
> r
```

```
13-letter RNAString object
seq: UUGAAAAA-CUC-N
```

```
> r == d
```

```
[1] TRUE
```

4 The *XStringViews* class and its subsetting operators [and [[

An *XStringViews* object contains a set of views *on the same XString* object called the *subject* string. Here is an *XStringViews* object with 4 views:

```
> v4 <- Views(dd2, start=3:0, end=5:8)
> v4
```

Views on a 6-letter DNAString subject

subject: -CTC-N

views:

| | start | end | width | |
|-----|-------|-----|-------|------------|
| [1] | 3 | 5 | 3 | [TC-] |
| [2] | 2 | 6 | 5 | [CTC-N] |
| [3] | 1 | 7 | 7 | [-CTC-N] |
| [4] | 0 | 8 | 9 | [-CTC-N] |

```
> length(v4)
```

```
[1] 4
```

Note that the 2 last views are *out of limits*.

You can select a subset of views from an *XStringViews* object:

```
> v4[4:2]
```

Views on a 6-letter DNAString subject

subject: -CTC-N

views:

| | start | end | width | |
|-----|-------|-----|-------|------------|
| [1] | 0 | 8 | 9 | [-CTC-N] |
| [2] | 1 | 7 | 7 | [-CTC-N] |
| [3] | 2 | 6 | 5 | [CTC-N] |

The returned object is still an *XStringViews* object, even if we select only one element. You need to use double-brackets to extract a given view as an *XString* object:

```
> v4[[2]]
```

5-letter DNAString object

seq: CTC-N

You can't extract a view that is *out of limits*:

```
> v4[[3]]
```

```
Error in getListElement(x, i, ...) : view is out of limits
```

Note that, when `start` and `end` are numeric vectors and `i` is a *single* integer, `Views(b, start, end)[[i]]` is equivalent to `subseq(b, start[i], end[i])`.

Subsetting also works with negative or logical values with the expected semantic (the same as for R built-in vectors):

```
> v4[-3]
```

Views on a 6-letter DNASTring subject

subject: -CTC-N

views:

| | start | end | width | |
|-----|-------|-----|-------|-----------|
| [1] | 3 | 5 | 3 | [TC-] |
| [2] | 2 | 6 | 5 | [CTC-N] |
| [3] | 0 | 8 | 9 | [-CTC-N] |

```
> v4[c(TRUE, FALSE)]
```

Views on a 6-letter DNASTring subject

subject: -CTC-N

views:

| | start | end | width | |
|-----|-------|-----|-------|-----------|
| [1] | 3 | 5 | 3 | [TC-] |
| [2] | 1 | 7 | 7 | [-CTC-N] |

Note that the logical vector is recycled to the length of `v4`.

5 A few more *XStringViews* objects

12 views (all of the same width):

```
> v12 <- Views(DNASTring("TAATAATG"), start=-2:9, end=0:11)
```

This is the same as doing `Views(d, start=1, end=length(d))`:

```
> as(d, "Views")
```

Hence the following will always return the `d` object itself:

```
> as(d, "Views")[[1]]
```

3 *XStringViews* objects with no view:

```
> v12[0]
```

```
> v12[FALSE]
```

```
> Views(d)
```

6 The == binary operator for *XStringViews* objects

This operator is the vectorized version of the == operator defined previously for *XString* objects:

```
> v12 == DNASTring("TAA")
```

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

To display all the views in v12 that are equals to a given view, you can type R cuties like:

```
> v12[v12 == v12[4]]
```

Views on a 8-letter DNASTring subject

subject: TAATAATG

views:

| | start | end | width | |
|-----|-------|-----|-------|-------|
| [1] | 1 | 3 | 3 | [TAA] |
| [2] | 4 | 6 | 3 | [TAA] |

```
> v12[v12 == v12[1]]
```

Views on a 8-letter DNASTring subject

subject: TAATAATG

views:

| | start | end | width | |
|-----|-------|-----|-------|-----|
| [1] | -2 | 0 | 3 | [] |
| [2] | 9 | 11 | 3 | [] |

This is TRUE:

```
> v12[3] == Views(RNASTring("AU"), start=0, end=2)
```

7 The start, end and width methods

```
> start(v4)
```

```
[1] 3 2 1 0
```

```
> end(v4)
```

```
[1] 5 6 7 8
```

```
> width(v4)
```

```
[1] 3 5 7 9
```

Note that `start(v4)[i]` is equivalent to `start(v4[i])`, except that the former will not issue an error if `i` is out of bounds (same for `end` and `width` methods).

Also, when `i` is a *single* integer, `width(v4)[i]` is equivalent to `length(v4[[i]])` except that the former will not issue an error if `i` is out of bounds or if view `v4[i]` is *out of limits*.