Vectorizing the DNAString function (work in progress)

Hervé Pagès

March 2, 2011

Contents

1	Introduction	1
2	DNAString vs XStringViews	1
3	The XStringViews generic function	2
4	Performance	2
5	Loading a FASTA file into an XStringViews object	3
6	Switching between DNA and RNA views	4

1 Introduction

This is a short tour on the DNAString function vectorization feature. Feel free to add your own comments.

2 DNAString vs XStringViews

The Biostrings2Classes vignette presents a proposal for 2 new classes (XString and XStringViews) as a replacement for the *BioString* class currently defined in the *Biostrings* 1 (*Biostrings* v 1.4.x) package.

It also shows how to use the DNAString function to create a DNAString object (a DNAString object is just a particular case of an XString object):

> d <- DNAString("TTGAAAA-CTC-N")
> is(d, "XString")

[1] TRUE

However this function is NOT vectorized: it always returns a *DNAString* object (which can only represent a *single* string).

In *Biostrings* 1, the DNAString function IS vectorized. Its vectorized form does the following: (1) concats the elements of its **src** argument into a single big string, (2) stores the offsets of all these elements in the **offsets** slot.

This behaviour is not immediatly obvious to the user, until he looks at the offsets slot.

It always returns a *BioString* object (with has as many values as the number of elements passed in the src argument).

3 The XStringViews generic function

The feature described in the previous section (provided by the vectorized form of the DNAString function in *Biostrings* 1) is provided in *Biostrings* 2 via the XStringViews generic function:

```
> v <- XStringViews(c("TTGAAAA-C", "TC-N"), "DNAString")
> v
Views on a 13-letter DNAString subject
subject: TTGAAAA-CTC-N
views:
   start end width
[1] 1 9 9 [TTGAAAA-C]
[2] 10 13 4 [TC-N]
```

4 Performance

The following example was provided by Wolfgang:

```
> library(hgu95av2probe)
```

```
> system.time(z <- XStringViews(hgu95av2probe$sequence, "DNAString"))</pre>
```

user system elapsed 0.200 0.008 0.208

> z

```
Views on a 5045000-letter DNAString subject
subject: TGGCTCCTGCTGAGGTCCCCTTTCCGGGCTG...CCCTCGTGCTCCTTGTCAACAGCGCACCCA
views:
```

	start	end	width	
[1]	1	25	25	[TGGCTCCTGCTGAGGTCCCCTTTCC]
[2]	26	50	25	[GGCTGTGAATTCCTGTACATATTTC]
[3]	51	75	25	[GCTTCAATTCCATTATGTTTTAATG]
[4]	76	100	25	[GCCGTTTGACAGAGCATGCTCTGCG]
[5]	101	125	25	[TGACAGAGCATGCTCTGCGTTGTTG]
[6]	126	150	25	[CTCTGCGTTGTTGGTTTCACCAGCT]
[7]	151	175	25	[GGTTTCACCAGCTTCTGCCCTCACA]

[8]	176	200	25	[TTCTGCCCTCACATGCACAGGGATT]
[9]	201	225	25	[CCTCACATGCACAGGGATTTAACAA]
•••	•••	• • •	•••	
[201792]	5044776	5044800	25	[GAGTGCCAATTCGATGATGAGTCAG]
[201793]	5044801	5044825	25	[ACACTGACACTTGTGCTCCTTGTCA]
[201794]	5044826	5044850	25	[CAATTCGATGATGAGTCAGCAACTG]
[201795]	5044851	5044875	25	[GACTTTCTGAGGAGATGGATAGCCT]
[201796]	5044876	5044900	25	[AGATGGATAGCCTTCTGTCAAAGCA]
[201797]	5044901	5044925	25	[ATAGCCTTCTGTCAAAGCATCATCT]
[201798]	5044926	5044950	25	[TTCTGTCAAAGCATCATCTCAACAA]
[201799]	5044951	5044975	25	[CAAAGCATCATCTCAACAAGCCCTC]
[201800]	5044976	5045000	25	[GTGCTCCTTGTCAACAGCGCACCCA]

With *Biostrings* 1, the call to DNAString(hgu95av2probe\$sequence) takes about 20 minutes... (the implementation of the vectorization feature is quadratic in time, as reported by Wolfgang).

5 Loading a FASTA file into an *XStringViews* object

The read.XStringViews function can be used to load a FASTA file in an XStringViews object:

```
> file <- system.file("extdata", "someORF.fa", package = "Biostrings")
> orf <- read.XStringViews(file, subjectClass = "DNAString")
> orf
```

[1]	1	5573	5573	[ACTTGTAAATATATCTTTTATTTTTATCGACCTTATTGTTGATAT]
[2]	5574	11398	5825	[TTCCAAGGCCGATGAATTCGACTGTAAATTTTTTTCTATTCTCTT]
[3]	11399	14385	2987	[CTTCATGTCAGCCTGCACTTCTGGGTACTCATGTAGCTGCCTCAT]
[4]	14386	18314	3929	[CACTCATATCGGGGGTCTTACTTGTCCCGAAACACGAAAAAGTAC]
[5]	18315	20962	2648	[AGAGAAAGAGTTTCACTTCTTGATATAATTTATGTGTGAACATAG]
[6]	20963	23559	2597	[GTGTCCGGGCCTCGCAGGCGTTCAGTTTTGGCAGAATGTACTTTT]
[7]	23560	26339	2780	[CAAGATAATGTCAAAGTTAGTGGCTAAGGAAGAAAAAAAAAA

```
> names(orf)
```

```
[1] "YALOO1C TFC3 SGDID:S000001, Chr I from 152168-146596, reverse complement, Verified ORF"
[2] "YALOO2W VPS8 SGDID:S000002, Chr I from 142709-148533, Verified ORF"
[3] "YALO03W EFB1 SGDID:S000003, Chr I from 141176-144162, Verified ORF"
[4] "YALO05C SSA1 SGDID:S000004, Chr I from 142433-138505, reverse complement, Verified ORF"
[5] "YALO07C ERP2 SGDID:S000005, Chr I from 139347-136700, reverse complement, Verified ORF"
[6] "YALO08W FUN14 SGDID:S000006, Chr I from 135916-138512, Verified ORF"
[7] "YALO09W SP07 SGDID:S000007, Chr I from 134856-137635, Verified ORF"
```

6 Switching between DNA and RNA views

The XStringViews function can also be used to switch between "DNA" and "RNA" views on the same string:

```
> orf2 <- XStringViews(orf, "RNAString")</pre>
```

These conversions are very fast because no string data needs to be copied:

```
> subject(orf)@shared
```

SharedRaw of length 26339 (data starting at address 0x98610b8)

> subject(orf2)@shared

SharedRaw of length 26339 (data starting at address 0x98610b8)