Object Oriented Microarray and Proteomics Analysis (OOMPA)

Kevin R. Coombes

May 6, 2019

Contents

1	Introduction	1
2	Getting Started	1
3	Color Schemes	2
4	Row-by-row Matrix Operations	2
5	Color Coded Graphs	5

1 Introduction

OOMPA is a suite of object-oriented tools for processing and analyzing large biological data sets, such as those arising from mRNA expression microarrays or mass spectrometry proteomics.

This vignette documents the base package, <code>compaBase</code>. A critical (but invisible to the user) feature of the <code>compaBase</code> package is that it defines a <code>class union</code> allowing you to use "numeric" or "NULL" objects in the design of an S4 class. More interesting user-visible features include alternative color schemes and vectorized matrix operations to speed the computation of row-by-row means, variances, and t-tests.

2 Getting Started

You invoke the package in the usual way:

> library(oompaBase)

3 Color Schemes

To illustrate the various color schemes, we first create a structured matrix:

```
> mat <- matrix(1:1024, ncol=1)
The following code is used to generate Figure 1.
> # windows(width=6,height=8)
> opar <- par(mfrow=c(6, 1), mai=c(0.3, 0.5, 0.2, 0.2))
> image(mat, col=redgreen(64), main='redgreen')
> image(mat, col=jetColors(128), main='jetColors')
> image(mat, col=blueyellow(32), main='blueyellow')
> image(mat, col=redscale(64), main='redscale')
> image(mat, col=bluescale(64), main='bluescale')
> image(mat, col=greyscale(64), main='greyscale')
> par(opar)
```

4 Row-by-row Matrix Operations

We now want to illustrate the "matrix operations" that allow for rapid computation of row-by-row means, variances, and t-tests.

We start by creating a slightly more interesting matrix full of random data. First, we make the variance larger in the second half (by column) of the data than in the first half.

```
> ng <- 10000
> ns <- 50
> dat <- matrix(rnorm(ng*ns, 0, rep(c(1, 2), each=25)), ncol=ns, byrow=TRUE)
Next, we shift the mean for the first 500 "genes" (rows).
> dat[1:500, 1:25] <- dat[1:500, 1:25] + 2</pre>
In order to compute t-tests, we also assign arbitrary labels separating the "sam-
ple columns" into two groups.
> clas <- factor(rep(c('Good', 'Bad'), each=25))</pre>
   Here we compute the row-by-row means.
> a0 <- proc.time()
> myMean <- matrixMean(dat)</pre>
> used0 <- proc.time() - a0
For comparison purposes, we perfor the same computation using apply.
> a1 <- proc.time()</pre>
> mm <- apply(dat, 1, mean)
> used1 <- proc.time() - a1
```

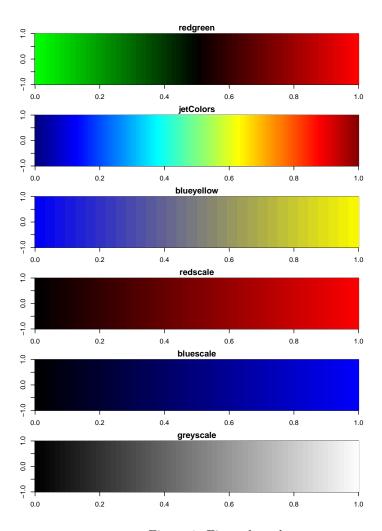


Figure 1: Five color schemes.

The results are the same, to within round-off error.

> summary(as.vector(myMean-mm))

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -8.882e-16 -2.776e-17 0.000e+00 -3.377e-19 2.776e-17 7.772e-16
```

There is a measurable (although not really user-perceptible) difference in the time for the two methods.

```
> used0

user system elapsed 0.00 0.01 0.02

> used1

user system elapsed 0.06 0.00 0.06
```

Here we compute the variances using two different methods.

```
> a0 <- proc.time()
> myVar <- matrixVar(dat, myMean)
> a1 <- proc.time()
> vv <- apply(dat, 1, var)
> a2 <- proc.time()</pre>
```

Again, the values are the same:

```
> summary(as.vector(myVar - vv))
```

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -4.441e-15 -4.441e-16 0.000e+00 2.875e-18 4.441e-16 4.885e-15
```

However, the time savings is substantially larger.

Not surprisingly, there is an even bigger time savings when computing (equal variance) t-statistics.

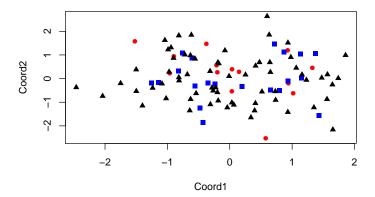
```
> t0 <- proc.time()
> myT <- matrixT(dat, clas)</pre>
> t1 <- proc.time()
> tt <- sapply(1:nrow(dat), function(i) {</pre>
    t.test(dat[i,clas=="Bad"], dat[i, clas=="Good"], var.equal=T)$statistic
+ })
> t2 <- proc.time()
> summary(as.vector(tt - myT))
              1st Qu.
                           Median
                                        Mean
                                                 3rd Qu.
                                                               Max.
-5.329e-15 -1.110e-16 0.000e+00 5.948e-18 1.110e-16 6.217e-15
> t1 - t0
   user system elapsed
              0
> t2 - t1
   user system elapsed
   1.87
           0.03
                   1.90
```

5 Color Coded Graphs

We frequently find ourselves producing multiple figures with a common color scheme, where each color or each symbol is used to denote samples or genes with a particular property (in the simplest case, "cancer" versus "normal"). Because we got tired of continually cutting and pasting plot and points commands and making sure the color legends stayed synchronized, we developed the ColorCoding and ColorCodedPair classes to encapsulate this notion.

We can simulate some data as an example.

```
> par(mfrow=c(2,1))
> plot(ColorCodedPair(x[,1], x[,2], codes), xlab="Coord1", ylab="Coord2")
> plot(ColorCodedPair(x[,1], x[,3], codes), xlab="Coord1", ylab="Coord3")
> par(mfrow=c(1,1))
```



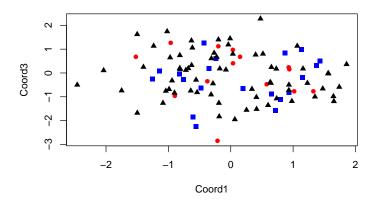


Figure 2: Color coded plots of three (simulated) related variables.