SVGMapping tutorial

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Abstract

Here we present how to use `SVGMapping`, an R package that aims at displaying experimental data on custom-made SVG images. For example, it allows you to create an image showing a cellular mechanism with relevant genes displayed as circles, and colored according to their expression level in a microarray experiment.

SVG is an image format that has the property of being vector-based, meaning that an SVG image can be scaled as big as you want without loosing quality. Moreover, it is becoming increasingly popular with the possibility to integrate SVG files in HTML (a new feature of HTML 5) and to dynamically modify SVG content using JavaScript. We suggest to create your SVG drawings by using the free Inkscape[1] software.

Contents

[1] http://inkscape.org/

1 Quickstart

First we need to load the library into the current workspace.

```
> library(SVGMapping)
```

During this tutorial we will use the sample data set provided with this package. This data set contains expression levels of a subset of genes taken from an experiment in which authors have measured the transcriptional response of *Saccharomyces cerevisiae* to aeration after anaerobic growth (the complete original data set is available on the GEO[2] website under the accession number GSE7140). It also contains a yeast genes annotation matrix. More details about these two variables will be given later in the tutorial.

```
> data(yeastExprData)       # Expression data from geo:GSE7140
> data(yeastAnnotMatrix)    # Annotations from SGD
```

Typical SVGMapping usage involves three steps. First, one has to load the source template. This is done using the loadSVG() function. On this example we will use a yeast TCA cycle pathway sketch.

```
> TCAtemplate <- system.file("extdata/example.svg", package="SVGMapping")
> mysvg <- loadSVG(TCAtemplate)
```

The second step concerns the data *mapping* itself. This task is done using the mapDataSVG() function. A key feature of this package is its ability to add multiple information on the same template by iteratively calling this function. On this very basic example only one call to this function will be necessary. Here expression log-ratios will be used to select background colors. Annotations with fold-change values will be used to build the javascript tooltip windows. Full details about the parameters of this function will be given in the next paragraphs.

```
> logratios <- yeastExprData[,1]
> foldchange <- ifelse(logratios>=0, 2^(logratios), -2^-logratios)
> mapDataSVG(mysvg,
+            numData=logratios,
+            tooltipData=foldchange,
+            annotation=yeastAnnotMatrix)
```

The last step is straightforward: we use the saveSVG() function to store the altered template on the filesystem. Here this will create a file named output1.svg inside the current directory. To view an SVG file, you can use a modern Web browser (*ie* compliant with the latest W3C standards) that supports the SVG image format. Safari 5.1, Firefox 5, Chrome 11 and Internet Explorer 9 are currently supported browsers that runs on Windows, OS/X and Linux. Another method is to use a dedicated drawing software such as Adobe Illustrator or Inkscape. Here one should see a drawing similar to the one on figure~1, with a tooltip window appearing when your mouse cursor is over the circles (MDH1 on this figure) that depict genes.

```
> saveSVG(mysvg, file="output1.svg")
```

Alternatively, one can call showSVG(mysvg) to automatically create a temporary file and open it in the default browser.

[2]http://www.ncbi.nlm.nih.gov/geo

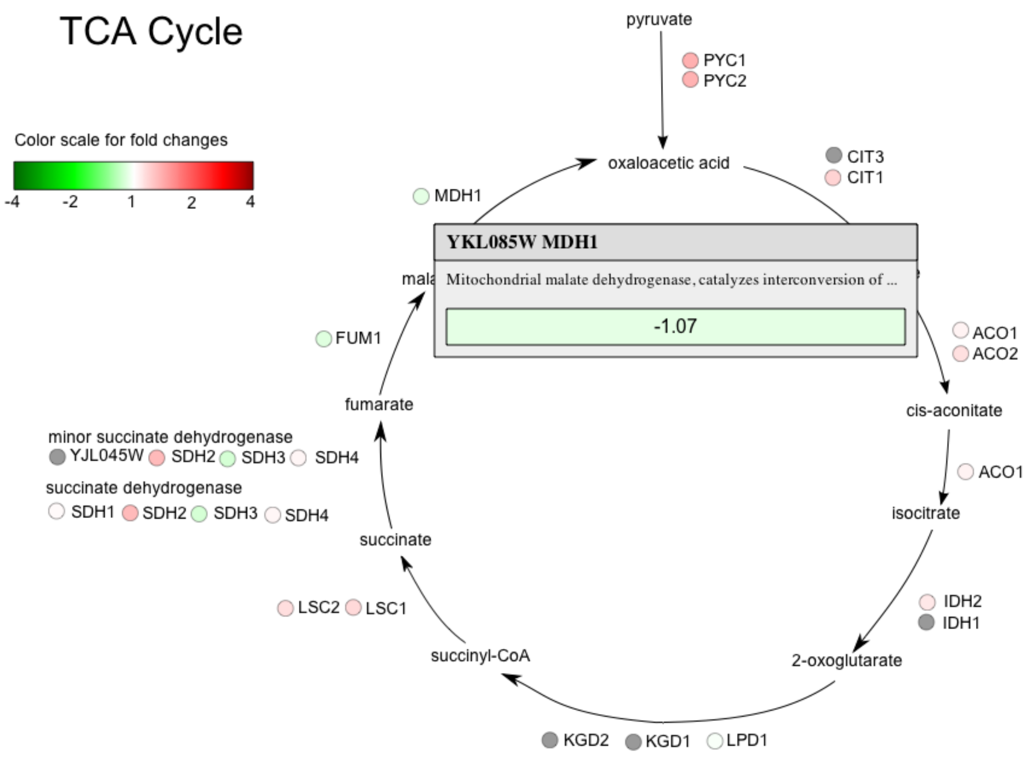


Figure 1: Screenshot of the produced “output1.svg” file

Hereafter we detail the template formatting and mapped data structure used to do this mapping . First, the template SVG file was created using Inkscape (a freely available program to edit SVG images). You retrieve the full path of the template using this command below.

```
> system.file("extdata/example.svg", package = "SVGMapping")
```

If you open this file with Inkscape, you’ll observe that, unlike the output file, circles for genes are all colored in grey. Remember that graphical shapes are identified using the *label* attributes. This attribute can be modified using the *object properties* dialog window (see the *Object* menu). If you open this window for grey circles you will notice labels related to yeast genes (*ie* YKL085W, YPL262W). SVGMapping uses these labels as a key index to select rows in the data matrix (*numData*) to retrieve expression values. For example, circles related to the genes MDH1 and FUM1 are labeled using related Orf names YKL085W and YPL262W. Thus, expression values using these Orf names will be used to select the corresponding color for filling the shape (this is the default action of the mapDataSVG() function). You can retrieve these expression values (as $\log_2(R/G)$) using:

```
> yeastExprData[c("YKL085W", "YPL262W"), 1]
```

```
   YKL085W    YPL262W
-0.1025448 -0.1268348
```

By default these values are converted to colors using a green-white-red gradient in the range $[-2, 2]$ (see the color scale on figure 1). You can customize the color scale and mapping range by passing optional arguments to mapDataSVG (more information on colors in section 5.1 on page˜11).

You can observe that the displayed value on the tooltip window for the `MDH1` gene (see figure 1) is -1.07 and differ from the value used to map colors -0.1025448. Indeed, we have proceeded to a systematic conversion of $\log_2(R/G)$ to fold changes using the formula:

$$\text{fold.change}(lgr) = \begin{cases} 2^{lgr} & \text{if } lgr \geq 0, \\ -2^{-lgr} & \text{otherwise} \end{cases}$$

We did this conversion because users sometimes prefer fold-changes over $\log_2$-ratios.

The other thing you can see on the tooltip is a name and description of the gene. This information is provided by the `annotation` parameter. In our example these annotations are taken from the `yeast2.db` R package˜[2], which we converted to a matrix. The content of the first three rows of this matrix is:

```
> substring(yeastAnnotMatrix[1:3, ], 0, 80)
```

```
        name
YAL001C "YAL001C TFC3"
YAL002W "YAL002W VPS8"
YAL003W "YAL003W EFB1"
        description
YAL001C "Largest of six subunits of the RNA polymerase III transcription initiation facto"
YAL002W "Membrane-associated protein that interacts with Vps21p to facilitate soluble vac"
YAL003W "Translation elongation factor 1 beta; stimulates nucleotide exchange to regenera"
        url
YAL001C "http://www.yeastgenome.org/cgi-bin/locus.fpl?locus=YAL001C"
YAL002W "http://www.yeastgenome.org/cgi-bin/locus.fpl?locus=YAL002W"
YAL003W "http://www.yeastgenome.org/cgi-bin/locus.fpl?locus=YAL003W"
```

As you can obsereve `yeastAnnotMatrix` is indexed by the same *labels* set in the SVG template. Besides the annotations displayed in the tooltip window, it contains an URL to redirect the navigator when clicking on gene circles[3].

2 Single condition modes

2.1 Line colors

It is possible to change line (stroke) colors, as illustrated by this example. Arrows were labeled using Inkscape with names like *'from-pyruvate'*. As you can see in the sample code below, by calling `mapDataSVG` several times it is possible to combine different information in the same file.

First we load the template:

```
> mysvg <- loadSVG(TCAtemplate)
```

Then, we color gene associated circles using expression levels (see section 1 on page˜2).

[3]In the example, URLs point to the "Saccharomyces Genome Database" website˜[1]

```
> mapDataSVG(mysvg,
+            numData=logratios,
+            tooltipData=foldchange,
+            annotation=yeastAnnotMatrix)
```

For each reaction, we assign an arbitrary "expression level" equal to the mean of the expression levels of the involved enzymes.

```
> reacdata <- c(mean(yeastExprData[c("YGL062W","YBR218C"),1]),
+                    yeastExprData["YKL085W",1],
+                    yeastExprData["YPL262W",1]
+               )
> names(reacdata) <- c("from-pyruvate",
+                      "from-malate",
+                      "from-fumarate")
```

The `reacdata` matrix is then used to map the **stroke** color of reaction lines, using the same color gradient as microarray (after removing lightest colors).

```
> mapDataSVG(mysvg,
+            numData=reacdata, mode="stroke",
+            tooltipData=NULL,
+            col=microarrayColors[c((1:333),(666:1000))])
```

Finally we save the modified SVG file in the current directory under the name *'output3.svg'* (see figure˜2).

```
> saveSVG(mysvg, file="output3.svg")
```

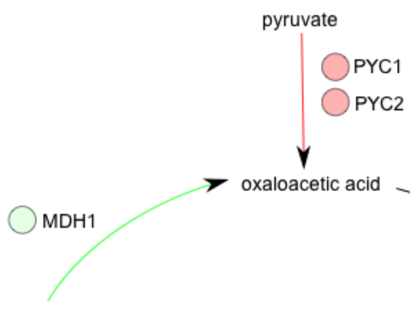


Figure 2: Screenshot of the produced "output3.svg" file

2.2 Filling Erlenmeyers

This package features a mode to display filled flasks where the liquid level is given in the data matrix, as a real number between 0 and 1. The following example illustrates this usage, and produces the result that can been seen on figure˜3 (the data used there is completely fake).

First we load a new template that contains the Erlenmeyers shapes besides the metabolites names.

```
> TCAtemplate2 <- system.file("extdata/example2.svg", package="SVGMapping")
> mysvg <- loadSVG(TCAtemplate2)
```

Our “fake” dataset contains “fake” metabolites concentration (in $mmol.l^{-1}$ unit) for “real” metabolites.

```
> mydata <- c(10, 25, 50)
> names(mydata) <- c("citrate", "cis-aconitate", "isocitrate")
```

The first `mapDataSVG()` instruction will set the filling colors and tooltips displayed values (*ie* we just add the unit).

```
> mapDataSVG(mysvg,
+            numData=mydata, mode="fill",
+            col=c("#FF0000","#00FF00","#0000FF"),
+            colrange=range(mydata),
+            tooltipData=paste(mydata, "mmol/L"))
```

The second `mapDataSVG()` instruction will set the filling heights using scaled values (in the range $[0, 1]$). Resulting image is saved in the current directory under the name *’output4.svg’* (see figure 3).

```
> mapDataSVG(mysvg,
+            numData=mydata/100, mode="partial-fill")
> saveSVG(mysvg, file="output4.svg")
```

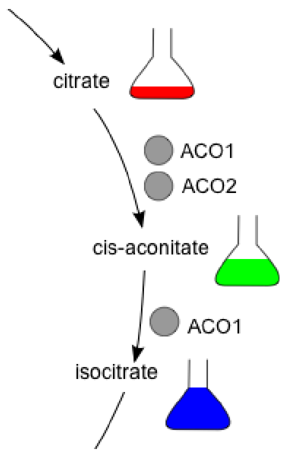


Figure 3: Screenshot of the produced “output4.svg” file

As you can see, it is possible to combine color change and filling level, but the color needs to be changed first. Indeed, the `partial-fill` mode will use the color defined by the `fill` mode.

Of course any SVG shape will work, so you can use this feature to simulate the filling of any closed graphical shape (*eg* battery energy level).

Note, however, that `SVGMapping` only defines the relative height, and does not know the surface which is actually filled, so depending on the shape, the surface filled will not necessarily be proportional to the value in the data matrix. It is your responsibility to apply a correction the numeric values if needed.

2.3 Other features

It is also possible to change opacity and line width, see the manual page of `mapDataSVG` for more information.

Functions are also provided if you want to manually edit the SVG data, see `setAttributeSVG` and `setStyleSVG`. As `SVGMapping` is built upon the XML R package, you can directly customize the SVG XML instructions.

3 Multi-conditions modes

3.1 Pie charts

Our program has a mode to replace circles by pie charts, with each slice corresponding to a different experiment. Here we illustrate this by showing expression data at different times (0, 5, 10, 20, 60, 120 minutes).

Let's load the TCA template previously used.

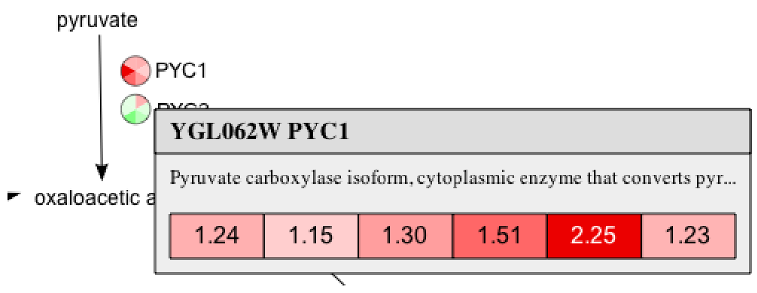
```
> mysvg <- loadSVG(TCAtemplate)
```

This time we will use all columns of the `yeastExprData` matrix (one column per time).

```
> logratios <- yeastExprData
> foldchange <- ifelse(logratios>=0, 2^(logratios), -2^-logratios)
```

Then we proceed as previously using the *pie* mode:

```
> mapDataSVG(mysvg,
+             numData=logratios, mode="pie",
+             tooltipData=foldchange,
+             annotation=yeastAnnotMatrix)
> saveSVG(mysvg, file="output2.svg")
```



YGL062W PYC1

Pyruvate carboxylase isoform, cytoplasmic enzyme that converts pyr...

1.24	1.15	1.30	1.51	2.25	1.23

Figure 4: Screenshot of the produced "output2.svg" file

Advice: To avoid confusing the user with many irrelevant colors, you might want to replace log-ratios that are not significant by zeros in order to have them displayed in white.

More advaned settings (like which section of the pie is the first value) are available. Pleaser refer to the mapDataSVG manual page.

3.2 Color stripes

An alternative to pie charts when comparing several experiments is to use color stripes. The following example illustrates this function and gives the result shown in figure˜5.

```
> mysvg <- loadSVG(TCAtemplate2)
> mydata <- matrix(c(-2, -1.5, -1, -0.5, 2, 1.5, 1, 0.5), ncol=4, byrow=TRUE)
> rownames(mydata) <- c("malate", "fumarate")
> mapDataSVG(mysvg, mydata, mode="fill")
> saveSVG(mysvg, file="output5.svg")
```

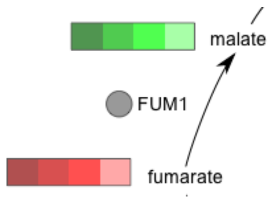


Figure 5: Screenshot of the produced "output5.svg" file

As you can see, no mode is specified so the *'fill'* mode is used by default. In the case of a multi-column data matrix, it will automatically switch to color stripes. It can be seen as a generalization of the *'fill'* mode.

4 Pseudo devices

Pseudo-device is a mechanism to include regular R graphics within a template. It allows to replace any rectangular shape with either the results of any set of R graphics commands or the content of any SVG file. In this section we will details both methods.

4.1 Substitute rectangular shapes with plots

As in all previous example we will start by loading a template. In this case it is a very sample sketch with one rectangle labelled *Rplot1*. The sketch is included in the package and can be loaded using:

```
> mysvg <- loadSVG(system.file("extdata/device-example.svg", package="SVGMapping"))
```

Next we open a new graphics device using the `devSVGMapping` function. This function has almost the same syntax as the SVG cairo driver. The only difference is that we specify a template and a target rectangular shape (given is attribute name and value). Given we use the *label* attribute to substitute the rectangle named *Rplot1* we declare our device using the following instruction:

```
> devSVGMapping(mysvg, "@inkscape:label", "Rplot1")
```

After this command all R graphics instruction will be *redirected* to the target shape. Internally, we open an SVG device to a temporary file.

As a example we can plot a heatmap of the first 30 genes expression levels of the previous microarrays yeast dataset:

```
> heatmap(yeastExprData[1:30, ], col = microarrayColors, labCol = NA,
+     scale = "none")
> dev.off()
```

Finally `dev.off` **must** be called to process and update the template. In practice the *real* SVG device is closed and the temporary output file included in the template using the `includeSVG` function (see below). The modified template is either saved (using `saveSVG`) or open in a web browser (using `showSVG`).

```
> saveSVG(mysvg, "pdev-output1.svg")
```

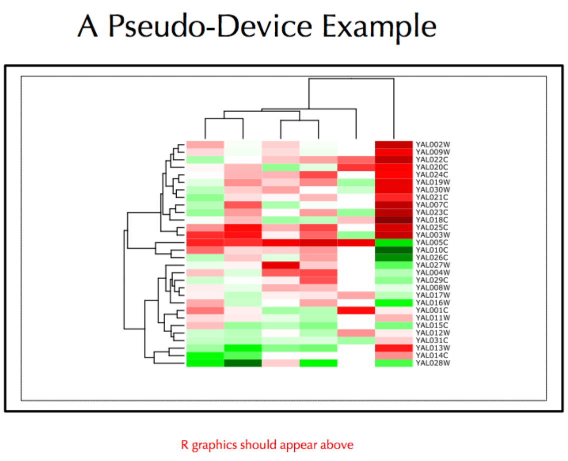


Figure 6: Screenshot of the produced “pdev-output1.svg” file

4.2 Include external SVG files

Another way to perform substitution within a SVG file is using the `includeSVG` function. The idea is the same as previously. First, we provide a pair of attributes name and values to identify a rectangular shape within the template. Second, the shape is substituted with the content of a given SVG file. Still, a scaling operation on the included file is perform to match the target area. Thus, one has to be very cautious about aspect ratio constraints.

As an illustratation of this function we will use the same template as above and fill the *Rplot1* area with a DNA replication sketch taken from *Wikimedia*.

```
> dna_svg <- "http://upload.wikimedia.org/wikipedia/commons/8/8f/DNA_replication_en.svg"
> mysvg <- loadSVG(system.file("extdata/device-example.svg", package = "SVGMapping"))
> includeSVG(template = mysvg, file = dna_svg, attribute.name = "@inkscape:label",
+     attribute.value = "Rplot1")
> saveSVG(mysvg, "pdev-output2.svg")
```

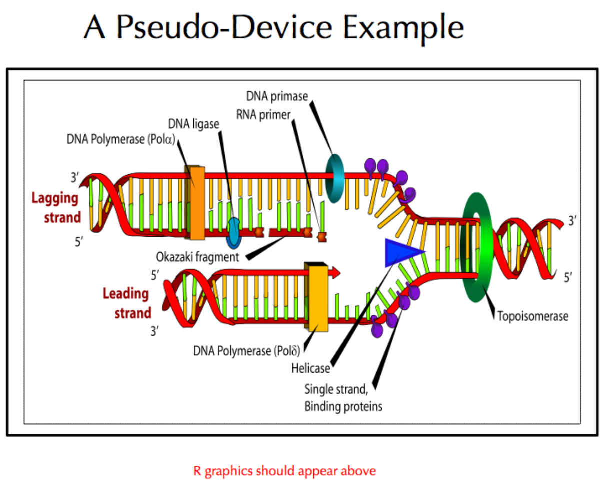


Figure 7: Screenshot of the produced "pdev-output2.svg" file

4.3 A more advanced example

The following example illustrates the use of several rectangles in which data is plotted using R and then included in the SVG file by SVGMapping.

```
> mysvg <- loadSVG(system.file("extdata/example3.svg", package = "SVGMapping"))
> genes <- getLabelsSVG(mysvg)
> genes <- genes[grepl("^Y.+\\-plot$", genes)]
> genes <- sapply(strsplit(genes, "-", fixed = TRUE), function(x) x[[1]])
> timeValues <- c(0, 5, 10, 20, 60, 120)
> for (gene in genes) {
+     devSVGMapping(mysvg, attribute.value = paste(gene, "-plot",
+         sep = ""), width = 1.5, height = 1)
+     par(mar = c(0, 0, 2, 0))
+     shortGeneName <- strsplit(yeastAnnotMatrix[gene, "name"],
+         " ", fixed = TRUE)[[1]]
+     shortGeneName <- shortGeneName[[length(shortGeneName)]]
+     ylims <- 1.2
+     image(c(timeValues[1], timeValues[length(timeValues)]), seq(-ylims,
+         ylims, length.out = 21), matrix(seq(-ylims, ylims, length.out = 20),
+         nrow = 1), col = microarrayColors, main = shortGeneName)
+     points(timeValues, yeastExprData[gene, ], type = "o")
+     dev.off()
+ }
> logratios <- yeastExprData
> mapDataSVG(mysvg, logratios, tooltipData = ifelse(logratios >=
+     0, 2^(logratios), -2^-logratios), mode = "pie", annotation = yeastAnnotMatrix)
> showSVG(mysvg)
```

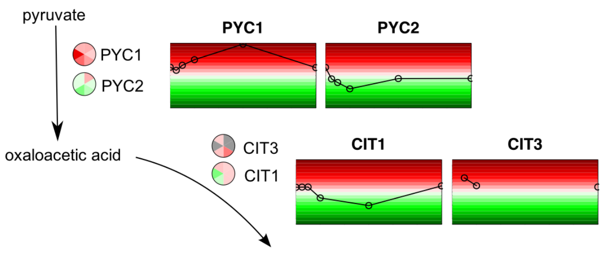


Figure 8: Each small plot shows the expression of a gene as a function of time. The plots are generated with R and are included in the SVG file with SVGMapping.

5 Advanced settings

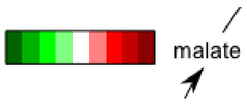
5.1 Colors

5.1.1 Changing the colors

All functions that produce colors in `mapDataSVG` call `computeExprColors` to compute colors from numeric data. This function uniformly maps a range $[a, b]$ to a list of colors, by making the assumption that the first color should be mapped to a and the last to b. When using `mapDataSVG`, these settings are called `col` and `colrange`. The default is $a = -2$ and $b = 2$.

If you want to display a continuous variable using colors, you need to provide a list of colors with a gradient containing all possible colors in your range. The default gradient, `microarrayColors`, contains 1000 colors that go from green to red (see figure˜1).

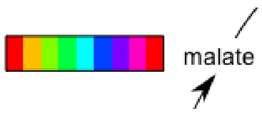
```
> mysvg <- loadSVG(TCAtemplate2)
> mapDataSVG(mysvg, matrix(seq(-2,2,by=0.5), nrow=1, dimnames=list("malate", NULL)))
> showSVG(mysvg)
```



You can specify a different list of colors. Note that it is recommended to provide a long list of colors so that `computeExprColors` can select the right colors with a maximum precision. A gradient with 1000 colors is a typical good length because it provides a high precision. Increasing it even more makes no sense since there is a finite number of possible colors in a computer, and a human being cannot make the difference between infinitely near colors.

On this example below we use a custom rainbow gradient rather than the default microarray green-white-red gradient.

```
> mysvg <- loadSVG(TCAtemplate2)
> mapDataSVG(mysvg, matrix(seq(-2,2,by=0.5), nrow=1, dimnames=list("malate", NULL)),
+             col=substring(rainbow(1000), 0, 7))
> showSVG(mysvg)
```

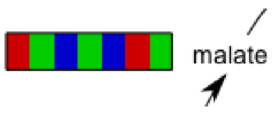


The substring call is required because the rainbow() function returns a list of colors in the #RRGGBBAA format while SVG uses the #RRGGBB format.

5.1.2 Discrete color mapping

You might also be interested in **discrete** color mapping (where colors are selected using their position in the *col* list):

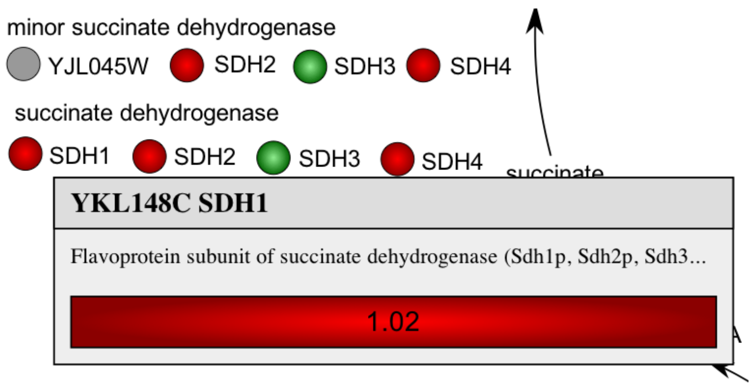
```
> mysvg <- loadSVG(TCAtemplate2)
> mapDataSVG(mysvg, matrix(c(1,2,3,2,3,1,2), nrow=1, dimnames=list("malate", NULL)),
+            col=c("#CC0000", "#00CC00", "#0000CC"), colrange=c(1,3))
> showSVG(mysvg)
```



5.1.3 Using gradients instead of colors

Instead of using colors, you may want to use references to gradients you declared. In this case the mapping is necessarily discrete, and only works in single-experiment fill mode.

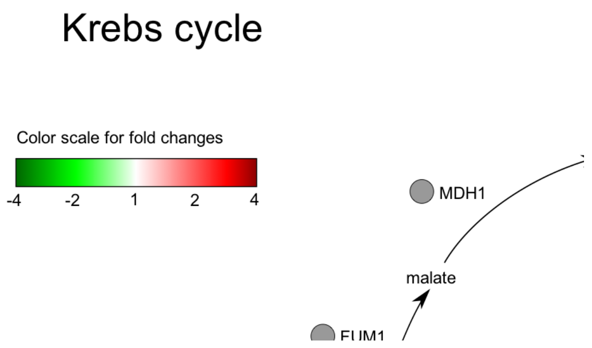
```
> mysvg <- loadSVG(TCAtemplate2)
> stop1 <- newXMLNode("stop", attrs=list(offset=0, style="stop-color:red"))
> stop2 <- newXMLNode("stop", attrs=list(offset=1, style="stop-color:darkred"))
> gradient <- newXMLNode("radialGradient", attrs=list(id="redGradient"),
+                        .children=list(stop1,stop2))
> addDefinesSVG(mysvg, gradient)
> stop1 <- newXMLNode("stop", attrs=list(offset=0, style="stop-color:lightgreen"))
> stop2 <- newXMLNode("stop", attrs=list(offset=1, style="stop-color:darkgreen"))
> gradient <- newXMLNode("radialGradient", attrs=list(id="greenGradient"),
+                        .children=list(stop1,stop2))
> addDefinesSVG(mysvg, gradient)
> logratios <- yeastExprData[,1]
> # Here log-ratios are used for colors but fold-changes are displayed
> mapDataSVG(mysvg, logratios, tooltipData=ifelse(logratios>=0, 2^(logratios), -2^-logratios),
+            annotation=yeastAnnotMatrix, col=c("url(#greenGradient)", "url(#redGradient)"))
> showSVG(mysvg)
```


minor succinate dehydrogenase
YJL045W
SDH2
SDH3
SDH4
succinate dehydrogenase
SDH1
SDH2
SDH3
SDH4
YKL148C SDH1
Flavoprotein subunit of succinate dehydrogenase (Sdh1p, Sdh2p, Sdh3...
1.02

5.2 Editing text content

You can use SVGMapping to dynamically change text content and add links. In the following example, we change the title from "TCA cycle" to "Krebs cycle", and add a link to the corresponding Wikipedia page.

```
> mysvg <- loadSVG(system.file("extdata/example.svg", package="SVGMapping"))
> setTextSVG(mysvg, "text3091", "Krebs cycle", searchAttribute="id")
> addLinkByLabelSVG(mysvg, "text3091", "http://en.wikipedia.org/wiki/TCA_cycle",
+                   searchAttribute="id")
> showSVG(mysvg)
```



5.3 Multiple object changes

If you want to apply SVGMapping several times to the same object, be careful. Some mapDataSVG modes only perform simple modifications (color change, opacity change) and can therefore be combined (you can call mapDataSVG several times to modify the same objects). But other more advanced modes, tipically those that create new SVG shapes (like pie, stripes, partial-fill), cannot be followed by other changes on the same objects. For example, if you want to have erlenmeyers filled with a color and level both depending on the data, you need to change the color and then set the filling level. Doing it the other way round will not work.

If you want to try strange combinations (combining stripes with partial-fill, or pie with partial-fill), please be aware that, although it might work, you cannot expect it to continue working it later releases of SVGMapping, as we don't include such cases in our tests.

If you want to do more complicated things that what we provide, keep in mind that SVGMapping is not a general SVG generation tool. However you might still find it useful as you can both use SVGMapping and modify the SVG (XML) tree manually using the R XML library (the object retruned by loadSVG is a modifiable XMLInternalDocument object from the R XML library).

References

[1] SGD project. ”Saccharomyces Genome Database” `http://downloads.yeastgenome.org/`.

[2] Marc Carlson, Seth Falcon, Herve Pages, and Nianhua Li. *yeast2.db: Affymetrix Yeast Genome 2.0 Array annotation data (chip yeast2).* R package version 2.4.5.