

Documentation of the RMAGEML package

Steffen Durinck^{‡,*}, Joke Allemeersch^{‡,†}, Vincent J Carey[¶], Yves Moreau[‡],
Bart De Moor[‡]

April 13, 2011

[‡]Department of Electronical Engineering, ESAT-SCD, K.U.Leuven,
Kasteelpark Arenberg 10, 3001 Leuven-Heverlee, Belgium,
<http://www.esat.kuleuven.ac.be/~dna/BioI>

and [¶]Channing Laboratory, Brigham and Women's Hospital, 75 Francis Street, Boston
02115, USA

Contents

| | | |
|----------|--|----------|
| 1 | Introduction | 2 |
| 2 | Prerequisites | 2 |
| 3 | Getting started | 3 |
| 4 | Import to marray packages | 3 |
| 4.1 | One step import and creation of an marrayRaw object from MAGE-ML files | 3 |
| 4.2 | Creation of a Gnames marrayInfo object | 7 |
| 4.3 | Creation of an marrayLayout object | 8 |
| 4.4 | Make an marrayRaw object | 9 |
| 5 | Import to limma package | 9 |
| 5.1 | One step import and creation of a limma RGList object from MAGE-ML files | 9 |
| 5.2 | Creating the genes dataframe of an RGList object | 12 |
| 5.3 | Make an RGList object | 12 |

*Steffen.Durinck@esat.kuleuven.ac.be

†Joke.Allemeersch@esat.kuleuven.ac.be

1 Introduction

MAGE-ML or Microarray Gene Expression Markup Language is a language designed to describe and exchange information about microarray experiments. MAGE-ML is based on XML and can describe microarray designs, microarray experiment setups, gene expression data, and data analysis results.

This package provides the link between MAGE-ML files and BioConductor. It gives the possibility to read in MAGE-ML files that describe cDNA microarray experiments. The functions convert the MAGE-ML files into the customary BioConductor objects (i.e., `marrayLayout`, `marrayInfo` and `marrayRaw` objects or `limma RGList` objects).

Here we give a short introduction to the Microarray and GeneExpression Object Model (MAGE-OM) and how we implemented the extraction of information necessary to make BioConductor objects. For a full description of MAGE-OM, we refer to the Gene Expression Specification: <http://www.omg.org/cgi-bin/doc?formal/03-02-03>.

The main classes of the MAGE object model are `BioSequence`, `QuantitationType`, `ArrayDesign`, `DesignElement`, `Array`, `BioMaterial`, `BioAssay`, `BioAssayData`, `Experiment`, `HigherLevelAnalysis`, `Protocol`, `Description`, `AuditAndSecurity`, `Measurement`, and `BioEvent`.

In MAGE-ML these translate into packages with the same name. The packages needed for building BioConductor objects are `BioAssayData`, `BioAssay`, `BioMaterial`, `BioSequence`, `ArrayDesign`, and `DesignElement`.

The `DesignElement` package contains a mapping of *Features*, which are the actual features present on the array, to *Reporters*, the reporter a feature represents. The `DesignElement` package also provides a mapping from *Reporters* to their corresponding *BioSequence* references. These *BioSequence* objects are characterized by their name and database entries in the `BioSequence` package. The `ArrayDesign` package contains information on the layout of the array. From this package, we can derive the position of each *Feature* on the array in terms of *Zone* (block or grid) and row and column within each *Zone*. The `BioAssayData` package describes the feature references that were assayed and the measured and derived *QuantitationTypes*. The `BioAssay` package describes the different steps in the microarray experiment. The last package used to make BioConductor objects is the `BioMaterial` package and describes how a sample is treated to obtain, for example, labeled samples used for hybridization.

2 Prerequisites

The RMAGEML package depends on SJava(>= 0.68) and a Java VM, e.g. j2resdk1.4.0. Other dependencies are as the Java-MAGEstk API and Java Xerces included in the package itself.

3 Getting started

Installing the package. The package can be installed as a normal R package: download the RMAGEML_2.0.4.tar.gz package and under Unix use the command

```
R CMD INSTALL RMAGEML_2.1.0.tar.gz.
```

The equivalent command for Windows is

```
Rcmd INSTALL RMAGEML_2.1.0.zip.
```

The package automatically loads the Biobase and marrayInput packages from BioConductor and the SJava libraries, so these should be installed as well.

Starting R. Before starting R one should be aware that the RMAGEML package uses SJava and that SJava requires to set the LD_LIBRARY_PATH environment variable before starting R.

Without setting this variable the package won't work

Loading the package. You can load the package into R by typing

```
> library(RMAGEML)
```

4 Import to marray packages

4.1 One step import and creation of an marrayRaw object from MAGE-ML files

In the marray packages of BioConductor the design of an array experiment is typically described by an `marrayLayout` and `marrayInfo` object. The function `importMAGEML` parses all MAGE-ML files present in the directory, which is given as a parameter to the function. From these files it creates an `marrayLayout` object, containing the Layout of one type of microarrays, and an `marrayInfo` object containing the gene names and database entries of the features spotted on the array. The name of the database to which the entries refer, is given in the 'notes' slot of the `Gnames` object. Next the function will extract the raw data values and output a complete *marrayRaw* object as a result.

The function can be tested on the MEXP-14 dataset. This example is available from Array-Express at <http://www.ebi.ac.uk/arrayexpress/>.

If one knows which *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types* are required, the import function can be used as:

```

> datadir <- system.file("MAGEMLdata", package = "RMAGEML")
> raw <- importMAGEML(directory = datadir, package = "marray",
+   arrayID = "A-MEXP-14", DED = "DED:707", QTD = "QTD:707",
+   name.Rf = "QT:F635 Mean", name.Rb = "QT:B635 Median", name.Gf = "QT:F532 Mean",
+   name.Gb = "QT:B532 Median")

```

- Java Virtual Machine is running -

parsing MAGEML files

making Layout and Gnames objects

Reading am2730miame.txt

Reading am2731miame.txt

Reading am2732m.txt

Reading am2736m.txt

Reading am2737m.txt

Reading tm1826m.txt

Reading tm1827m.txt

Reading tm1829m.txt

Reading tm1830m.txt

Reading tm1831m.txt

```

> print(raw)

```

An object of class "marrayRaw"

@maRf

```

      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,] 5841 2030 2968  45 1828 1975 2077 1775 2202  841
[2,] 2002 1312  421  96  399  557  295  748  465   83
[3,] 2254 2057 1097 1163  649  917  755 1276  985  335
[4,] 2212 1492  782  767  709 1114  620 1004  860  488
[5,]  73  76  42  54  45  49  49  46  47  43
955 more rows ...

```

@maGf

```

      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]  852  750 1587  135 1625 1183 1598 1108  807 1746
[2,]  652  529  404  162  397  515  285  390  291  190
[3,]  576  615  634  386  734  820  696  573  457  572
[4,]  781  589  733  366  758  848  667  597  559  716
[5,]  157  143  111  124  130  148  135  137  146  131
955 more rows ...

```

@maRb

```

      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]

```

```
[1,] 42 42 36 39 41 47 40 45 49 42
[2,] 41 41 35 39 40 45 39 43 42 41
[3,] 41 42 34 41 40 44 40 43 42 42
[4,] 41 40 34 41 40 43 39 43 41 41
[5,] 41 39 34 40 40 42 39 43 41 41
```

955 more rows ...

@maGb

```
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,] 150 130 87 120 104 135 117 137 168 127
[2,] 147 128 88 111 105 136 116 131 137 121
[3,] 140 124 85 106 105 133 116 128 135 121
[4,] 138 122 88 108 106 133 116 128 134 120
[5,] 138 122 87 106 104 133 114 128 133 118
```

955 more rows ...

@maW

<0 x 0 matrix>

@maLayout

An object of class "marrayLayout"

@maNgr

[1] 4

@maNgc

[1] 4

@maNsr

[1] 10

@maNsc

[1] 6

@maNspots

[1] 960

@maSub

[1] TRUE

@maPlate

factor(0)

Levels:

@maControls

factor(0)

Levels:

@maNotes

[1] ""

@maGnames

An object of class "marrayInfo"

@maLabels

[1] "none" "none" "none" "none" "none"

955 more elements ...

@maInfo

[1] aj508733 V00618 aj291984 aj306233 aj310439

142 Levels: V00618 af025843 af034412 af135499 aj132353 aj291832 ... y17187

955 more rows ...

@maNotes

[1] "Identifiers refer to database: DB:embl"

@maTargets

An object of class "marrayInfo"

@maLabels

[1] "am2730miame.txt" "am2731miame.txt" "am2732m.txt" "am2736m.txt"

[5] "am2737m.txt" "tm1826m.txt" "tm1827m.txt" "tm1829m.txt"

[9] "tm1830m.txt" "tm1831m.txt"

@maInfo

Cy3 Cy5

1 AM-Pool AM2730-I

2 AM-Pool AM2731-1

3 AM-Pool AM2732-I

4 AM-Pool AM2736-I

5 AM-Pool AM2737-I

6 AM-Pool TM1826-I

7 AM-Pool TM1827-I

8 AM-Pool TM1829-I

9 AM-Pool TM1830-I

10 AM-Pool TM1831-I

```
@maNotes  
[1] "Description of the targets"
```

```
@maNotes  
character(0)
```

If however you do not know which *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types* to use, you can call the function as follows:

```
> datadir <- system.file("MAGEMLdata", package = "RMAGEML")  
> if (interactive()) {  
+   raw <- importMAGEML(directory = datadir, package = "marray")  
+ }
```

This will generate a few selection panels which allow selection of the appropriate *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types*.

4.2 Creation of a Gnames marrayInfo object

If one just wants to make an marrayInfo object containing the gene names and database identifiers of the spotted features the function getGnames can be used.

```
> data <- system.file("MAGEMLdata", package = "RMAGEML")  
> mageom <- importMAGEOM(directory = data)
```

parsing MAGEML files

```
> getGnames(mageom, arrayID = "A-MEXP-14", DED = "DED:707", package = "marray")
```

An object of class "marrayInfo"

```
@maLabels  
[1] "none" "none" "none" "none" "none"  
955 more elements ...
```

```
@maInfo  
[1] aj508733 V00618 aj291984 aj306233 aj310439  
142 Levels: V00618 af025843 af034412 af135499 aj132353 aj291832 ... y17187  
955 more rows ...
```

```
@maNotes  
[1] "Identifiers refer to database: DB:embl"
```

Again leaving out the 'DED' parameter will cause selection panels to pop up displaying the available *DesignElement Dimensions*.

4.3 Creation of an marrayLayout object

In the marray packages the information on the array layout is stored in an marrayLayout object which can be created by the getArrayLayout function.

```
> data <- system.file("MAGEMLdata", package = "RMAGEML")
> mageom <- importMAGEOM(directory = data)
```

parsing MAGEML files

```
> getArrayLayout(mageom, arrayID = "A-MEXP-14", DED = "DED:707")
```

An object of class "marrayLayout"

@maNgr

[1] 4

@maNgc

[1] 4

@maNsr

[1] 10

@maNsc

[1] 6

@maNspots

[1] 960

@maSub

[1] TRUE

@maPlate

factor(0)

Levels:

@maControls

factor(0)

Levels:

@maNotes

[1] ""

4.4 Make an marrayRaw object

The function `makeMarrayRaw` takes a `Gnames` and `Layout` object and parameters corresponding to the *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types* to create an *marrayRaw* object.

```
> data <- system.file("MAGEMLdata", package = "RMAGEML")
> mageom <- importMAGEOM(directory = data)

parsing MAGEML files

> gnames <- getGnames(mageom, arrayID = "A-MEXP-14", DED = "DED:707",
+   package = "marray")
> layout <- getArrayLayout(mageom, arrayID = "A-MEXP-14", DED = "DED:707")
> raw <- makeMarrayRaw(mageOM = mageom, layout = layout, gnames = gnames,
+   directory = data, arrayID = "A-MEXP-14", DED = "DED:707",
+   QTD = "QTD:707", name.Rf = "QT:F635 Mean", name.Rb = "QT:B635 Median",
+   name.Gf = "QT:F532 Mean", name.Gb = "QT:B532 Median")
```

```
Reading am2730miame.txt
Reading am2731miame.txt
Reading am2732m.txt
Reading am2736m.txt
Reading am2737m.txt
Reading tm1826m.txt
Reading tm1827m.txt
Reading tm1829m.txt
Reading tm1830m.txt
Reading tm1831m.txt
```

5 Import to limma package

5.1 One step import and creation of a limma RGList object from MAGE-ML files

In the `limma` package of `BioConductor` the raw data is stored in an `RGList` object. The function `importMAGEML` parses all MAGE-ML files present in the directory which is given as a parameter to the function. From these files it creates the `RGList` object, containing the layout, gene names and database entries of the features spotted on the array and the foreground and background intensities for the green and red channels.

The function can be tested on the MEXP-14 dataset. This example is available from Array-Express at <http://www.ebi.ac.uk/arrayexpress/>.

For import to `limma` the same function as `MAGEML` import to `marray` packages can be used, just adapt the name of the package into `limma` as follows:

```

> datadir <- system.file("MAGEMLdata", package = "RMAGEML")
> raw <- importMAGEML(directory = datadir, package = "limma", arrayID = "A-MEXP-14",
+   DED = "DED:707", QTD = "QTD:707", name.Rf = "QT:F635 Mean",
+   name.Rb = "QT:B635 Median", name.Gf = "QT:F532 Mean", name.Gb = "QT:B532 Median")

```

```

parsing MAGEML files
Reading am2730miame.txt
Reading am2731miame.txt
Reading am2732m.txt
Reading am2736m.txt
Reading am2737m.txt
Reading tm1826m.txt
Reading tm1827m.txt
Reading tm1829m.txt
Reading tm1830m.txt
Reading tm1831m.txt

```

```

> print(raw)

```

An object of class "RGList"

\$R

| | am2730miame.txt | am2731miame.txt | am2732m.txt | am2736m.txt | am2737m.txt |
|------|-----------------|-----------------|-------------|-------------|-------------|
| [1,] | 5841 | 2030 | 2968 | 45 | 1828 |
| [2,] | 2002 | 1312 | 421 | 96 | 399 |
| [3,] | 2254 | 2057 | 1097 | 1163 | 649 |
| [4,] | 2212 | 1492 | 782 | 767 | 709 |
| [5,] | 73 | 76 | 42 | 54 | 45 |

| | tm1826m.txt | tm1827m.txt | tm1829m.txt | tm1830m.txt | tm1831m.txt |
|------|-------------|-------------|-------------|-------------|-------------|
| [1,] | 1975 | 2077 | 1775 | 2202 | 841 |
| [2,] | 557 | 295 | 748 | 465 | 83 |
| [3,] | 917 | 755 | 1276 | 985 | 335 |
| [4,] | 1114 | 620 | 1004 | 860 | 488 |
| [5,] | 49 | 49 | 46 | 47 | 43 |

955 more rows ...

\$G

| | am2730miame.txt | am2731miame.txt | am2732m.txt | am2736m.txt | am2737m.txt |
|------|-----------------|-----------------|-------------|-------------|-------------|
| [1,] | 852 | 750 | 1587 | 135 | 1625 |
| [2,] | 652 | 529 | 404 | 162 | 397 |
| [3,] | 576 | 615 | 634 | 386 | 734 |
| [4,] | 781 | 589 | 733 | 366 | 758 |
| [5,] | 157 | 143 | 111 | 124 | 130 |

| | tm1826m.txt | tm1827m.txt | tm1829m.txt | tm1830m.txt | tm1831m.txt |
|--|-------------|-------------|-------------|-------------|-------------|
|--|-------------|-------------|-------------|-------------|-------------|

| | | | | | |
|------|------|------|------|-----|------|
| [1,] | 1183 | 1598 | 1108 | 807 | 1746 |
| [2,] | 515 | 285 | 390 | 291 | 190 |
| [3,] | 820 | 696 | 573 | 457 | 572 |
| [4,] | 848 | 667 | 597 | 559 | 716 |
| [5,] | 148 | 135 | 137 | 146 | 131 |

955 more rows ...

\$Rb

| | | | | | |
|------|-----------------|-----------------|-------------|-------------|-------------|
| | am2730miame.txt | am2731miame.txt | am2732m.txt | am2736m.txt | am2737m.txt |
| [1,] | 42 | 42 | 36 | 39 | 41 |
| [2,] | 41 | 41 | 35 | 39 | 40 |
| [3,] | 41 | 42 | 34 | 41 | 40 |
| [4,] | 41 | 40 | 34 | 41 | 40 |
| [5,] | 41 | 39 | 34 | 40 | 40 |

| | | | | | |
|------|-------------|-------------|-------------|-------------|-------------|
| | tm1826m.txt | tm1827m.txt | tm1829m.txt | tm1830m.txt | tm1831m.txt |
| [1,] | 47 | 40 | 45 | 49 | 42 |
| [2,] | 45 | 39 | 43 | 42 | 41 |
| [3,] | 44 | 40 | 43 | 42 | 42 |
| [4,] | 43 | 39 | 43 | 41 | 41 |
| [5,] | 42 | 39 | 43 | 41 | 41 |

955 more rows ...

\$Gb

| | | | | | |
|------|-----------------|-----------------|-------------|-------------|-------------|
| | am2730miame.txt | am2731miame.txt | am2732m.txt | am2736m.txt | am2737m.txt |
| [1,] | 150 | 130 | 87 | 120 | 104 |
| [2,] | 147 | 128 | 88 | 111 | 105 |
| [3,] | 140 | 124 | 85 | 106 | 105 |
| [4,] | 138 | 122 | 88 | 108 | 106 |
| [5,] | 138 | 122 | 87 | 106 | 104 |

| | | | | | |
|------|-------------|-------------|-------------|-------------|-------------|
| | tm1826m.txt | tm1827m.txt | tm1829m.txt | tm1830m.txt | tm1831m.txt |
| [1,] | 135 | 117 | 137 | 168 | 127 |
| [2,] | 136 | 116 | 131 | 137 | 121 |
| [3,] | 133 | 116 | 128 | 135 | 121 |
| [4,] | 133 | 116 | 128 | 134 | 120 |
| [5,] | 133 | 114 | 128 | 133 | 118 |

955 more rows ...

\$genes

| | Block | Row | Column | ID | Name |
|---|-------|-----|--------|----------|------|
| 1 | 1 | 1 | 1 | aj508733 | none |
| 2 | 1 | 1 | 2 | V00618 | none |
| 3 | 1 | 1 | 3 | aj291984 | none |

```

4      1      1      4 aj306233 none
5      1      1      5 aj310439 none
955 more rows ...

```

Similarly if one only specifies the ‘directory’ and the ‘package’, selection panels will pop up to select the *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types*.

5.2 Creating the genes dataframe of an RGList object

In limma the gene names, gene identifiers and layout information is stored in a dataframe which can be created by the `getArrayLayoutLimma` function.

```

> data <- system.file("MAGEMLdata", package = "RMAGEML")
> mageom <- importMAGEOM(directory = data)

```

parsing MAGEML files

```

> genes <- getArrayLayoutLimma(mageom, arrayID = "A-MEXP-14", DED = "DED:707")
> print(genes[1:10, ])

```

| | Block | Row | Column | ID | Name |
|----|-------|-----|--------|----------|------|
| 1 | 1 | 1 | 1 | aj508733 | none |
| 2 | 1 | 1 | 2 | V00618 | none |
| 3 | 1 | 1 | 3 | aj291984 | none |
| 4 | 1 | 1 | 4 | aj306233 | none |
| 5 | 1 | 1 | 5 | aj310439 | none |
| 6 | 1 | 1 | 6 | aj409363 | none |
| 7 | 1 | 1 | 7 | aj310516 | none |
| 8 | 1 | 1 | 8 | aj306230 | none |
| 9 | 1 | 1 | 9 | aj310436 | none |
| 10 | 1 | 1 | 10 | aj291834 | none |

5.3 Make an RGList object

The function `makeRG` takes a genes dataframe (containing the layout, gene identifiers and gene names), and parameters corresponding to *DesignElement Dimension*, *QuantitationType Dimension* and *Quantitation Types* to create a limma `RGList` object.

```

> data <- system.file("MAGEMLdata", package = "RMAGEML")
> mageom <- importMAGEOM(directory = data)

```

parsing MAGEML files

```
> genes <- getArrayLayoutLimma(mageom, arrayID = "A-MEXP-14", DED = "DED:707")
> raw <- makeRG(mageOM = mageom, genes = genes, directory = data,
+   arrayID = "A-MEXP-14", DED = "DED:707", QTD = "QTD:707",
+   name.Rf = "QT:F635 Mean", name.Rb = "QT:B635 Median", name.Gf = "QT:F532 Mean",
+   name.Gb = "QT:B532 Median")
```

Reading am2730miame.txt

Reading am2731miame.txt

Reading am2732m.txt

Reading am2736m.txt

Reading am2737m.txt

Reading tm1826m.txt

Reading tm1827m.txt

Reading tm1829m.txt

Reading tm1830m.txt

Reading tm1831m.txt