

eSet metadata structures

VJ Carey <stvjc@channing.harvard.edu>

May 18, 2005

1 Introduction

Metadata is data about data. In bioinformatics there are many roles for the metadata concept. This document describes management of metadata on the central data objects of downstream analysis of high-throughput data structures in Bioconductor. Specifically, the *exprSet* and *eSet* classes provide data structure conventions for collections of microarray experiments. These classes can be used to deal with data from other experimental paradigms. For this to occur, metadata conventions will be required so that the different components of the experimental data are identifiable programatically.

As a simple example, consider the recording of patient age. Information on age will be stored in a *phenoData* variable. For some studies, age is recorded in months; for others, age is recorded in years; and in others, age must be coarsened, and is recorded as a categorical response. It is not sufficient to record the age as a numeric variable named “age”. One may encode the units of age in the variable name, but a convention for decoding the name may be hard to specify conveniently.

Metadata structures and conventions can help to achieve standards for representation and decoding of data. To continue with the example, we use the *eset* example data.

```
> library(Biobase)
```

```
> data(eset)
```

```
> eset
```

```
Expression Set (exprSet) with
```

```
500 genes
```

```
26 samples
```

```
    phenoData object with 3 variables and 26 cases
```

```
varLabels
```

```
  cov1: Covariate 1; 2 levels
```

```
  cov2: Covariate 2; 2 levels
```

```
  cov3: Covariate 3; 3 levels
```

We will extract the *phenoData* component:

```
> pes <- phenoData(eset)
```

A utility called `convertVarLabels` will upgrade the *phenoData* component so that a general metadata container is present.

```
> pes <- convertVarLabels(pes)
> varMetadata(pes)
```

```
  varName      varLabels
1   cov1 Covariate 1; 2 levels
2   cov2 Covariate 2; 2 levels
3   cov3 Covariate 3; 3 levels
```

Arbitrarily many metadata entries may be added for any variable.

```
> pes <- addVarMetadataEntry(pes, "cov1", "units", "inches")
```

The specific metadata attribute “units” can be ascertained at the *phenoData* level:

```
> getUnits(pes, "cov1")
```

```
[1] inches
Levels: inches
```

The metadata container is currently a `data.frame`. For very general programmatic manipulation of metadata, XML or RDF representations may be desirable. Conversion from `data.frame` to XML may use the `StatDataML` package or other routines.

2 Details on *phenoData* metadata

At the *phenoData* level, a slot called `varMetadata` holds a `data.frame` instance. Currently there is no validation, but it seems reasonable that a `varMetadata` `data.frame` should have one row for each *phenoData* variable. Note that the typical reference of the term “variable” is a column of a data frame. For metadata, the variables define rows of the `varMetadata` container, and variable attributes or properties define the columns of the `varMetadata` container.

An informally reserved attribute name is `varName`. This is used to name the column that holds the names of variables in the *phenoData* `pData` component. The attribute name `verb+units+` is recognized by a helper method “`getUnits`”.

Any legacy *exprSet* instance can be converted to one with a `varMetadata` container using the `convertVarLabels` helper method. This places the *phenoData* `varLabels` content in a `data.frame` column named `varLabel1`. Ultimately the `varLabels` component of *phenoData* may be eliminated in favor of `varMetadata` conventions.

3 Details on the eMetadata container for eSet objects

The *exprSet* class has proven useful for affymetrix data representation. A new class, *eSet*, allows more complex data representation.

```
> getSlots("eSet")
```

```
      eList   phenoData  
"exprList" "phenoData"
```

```
> getSlots("exprList")
```

```
      .Data   eMetadata  
"exprListNM" "data.frame"
```

```
> getClass("exprListNM")
```

```
Extended class definition ( "ClassUnionRepresentation" )  
Virtual Class
```

```
No Slots, prototype of class "NULL"
```

```
Known Subclasses: "list", "environment", "exprList"
```

The *exprListNM* class has some legacy (under the name “*exprList*”) in Biobase, and is extended by the metadata-equipped *exprList* class. The *eMetadata* slot is for a container for metadata about the various components of the *exprList*. The current container class is *data.frame*. For a standard *exprSet* like *golubTrain*, this *data.frame* would have one row. An informally privileged attribute is “*name*”. The *getExpData* method looks for an *exprList* component named *exprs*, so the “*name*” attribute should have value *exprs* for this component.

The following shows the basic manipulations currently available; see the *eSet* class man page for additional methods.

```
> data(eset)
```

```
> md <- data.frame(name = "exprs", etype = "random numbers")
```

```
> newe <- new("exprList", .Data = list(exprs = exprs(eset)), eMetadata = md)
```

```
> es1 <- new("eSet", eList = newe, phenoData = phenoData(eset))
```

```
> es1
```

```
New Expression Set (eSet) with
```

```
  500 genes
```

```
  26 samples
```

```
          phenoData object with 3 variables and 26 cases
varLabels
  cov1: Covariate 1; 2 levels
  cov2: Covariate 2; 2 levels
  cov3: Covariate 3; 3 levels
```

```
> eMetadata(es1)
```

```
  name          etype
1 exprs random numbers
```

```
> eList(es1)
```

```
exprList object with 1 list element(s).
```

```
exprList level metadata:
```

```
  name          etype
1 exprs random numbers
```

Additional conventions should be established for multicolor arrays and other platforms.