

# Introduction to the xps Package: Classes structure

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## 1 Introduction

This document provides a tutorial on the class structures used in the `xps` package. The `xps` package provides S4 class definitions and associated methods for raw intensity data, preprocessed intensity data, expression measures, and detection call data for batches of Affymetrix expression or exon arrays. Detailed information on functions, classes and methods can be obtained in the help files.

Since the main purpose of the S4 classes is to provide a link to and allow access to `ROOT` files and the `ROOT` trees contained therein, it is important to understand the meaning of `ROOT` files and the `ROOT` trees first.

## 2 XPS and ROOT

Package `xps` is based on two powerful frameworks, namely `R` and `ROOT`. `ROOT`(<http://root.cern.ch>) is an object-oriented C++ framework that has been developed at CERN for distributed data warehousing

and data mining of particle data in the petabyte range. Data are stored as sets of objects in machine-independent files, and a specialized class, called a ROOT tree, has been designed to store large quantities of data, see The ROOT team (2009).

## 2.1 ROOT File

A ROOT file, C++ class *TFile*, is like a UNIX file directory. It can contain directories and objects organized in unlimited number of levels. It is also stored in machine independent format. Thus it can be considered to be the ROOT equivalent of an R `environment`. Just like an R `environment` a ROOT file can be copied to any system directory and used from within any OS.

A ROOT file can store any C++ object like ROOT trees, but also any other object such as a text file. For our purpose it is only important to know that ROOT trees can be stored in ROOT files.

## 2.2 ROOT Tree

ROOT trees, C++ class *TTree*, have been especially designed to store large quantities of same-class objects. As simplest case, a ROOT tree can store data imported from tables, and thus can be considered to be the ROOT equivalent of an R `data.frame`. A ROOT tree consists of branches and leaves, with each leaf containing the data from one column of the imported data table.

The *TTree* class is optimized to reduce disk space and enhance access speed. When using a TTree, you fill its branch buffers with leaf data and the buffers are written to disk when it is full. Branches, buffers, and leaves are explained in: The ROOT team (2009); here it is important to realize that each object is not written individually, but rather collected and written a bunch at a time. This is where *TTree* takes advantage of compression and will produce a much smaller file than if the objects were written individually.

## 3 XPS S4 classes

Taking advantage of the features described above, package `xps` stores all data as ROOT trees in portable ROOT files. The four main classes for Affymetrix oligonucleotide array data are:

**SchemeTreeSet:** Data describing microarray layout, probe information and metadata for genes are stored as ROOT trees in ROOT *scheme* files, accessible from R as S4 class *SchemeTreeSet* objects.

**DataTreeSet:** This class provides the link to ROOT data files and the ROOT trees contained therein. Data files contain the content of the raw CEL-files as ROOT trees. Additional data files can contain the background-corrected intensities as well as the computed background intensities.

**ExprTreeSet:** Preprocessing of raw data, i.e. summarization and normalization, results in conversion of probe level data to expression values. These data are stored as ROOT trees in ROOT expression files. Class *ExprTreeSet* provides the link to the ROOT expression file and the ROOT trees contained therein.

**CallTreeSet:** Results of MAS5 detection calls or DABG calls, respectively, and the corresponding p-values are stored as ROOT trees in ROOT call files, accessible via class *CallTreeSet*.

In addition, an extra S4 class exists for quality control:

**QualTreeSet:** This class provides the link to the ROOT quality control file and the ROOT trees contained therein.

All of these S4 classes are derived from the same virtual base class *TreeSet*.

The following classes are relevant for filtering and analysis of expression values:

**PreFilter:** This class allows the initialization of different non-specific filters and stores the relevant parameters of each filter.

**UniFilter:** This class allows the initialization of different univariate filters and stores the relevant parameters of each filter..

**FilterTreeSet:** This class provides a link between class *ExprTreeSet*, the filter class applied to this *ExprTreeSet* and the resulting ROOT filter file and the ROOT mask tree contained therein.

**AnalysisTreeSet:** Univariate analysis allows the selection of differentially expressed genes. This class provides a link between class *FilterTreeSet* containing the relevant filtering information, and the resulting ROOT filter file and the ROOT trees contained therein.

The S4 classes *PreFilter* and *UniFilter* are derived from base class *Filter* while S4 classes *FilterTreeSet* and *AnalysisTreeSet* are derived from the virtual base class *TreeSet*.

An optional S4 class, called *ProjectInfo*, can be used to describe the relevant phenotypic and MIAME-like project information.

### 3.1 TreeSet class

This is the virtual base class for all other S4 classes and provides the link to the ROOT file and the ROOT trees contained therein for the corresponding subclass.

Function `getClassDef` can be used to get information on the slots and the inheritance information:

```
> library(xps)
```

```
> getClassDef("TreeSet")
```

```
Virtual Class "TreeSet" [package "xps"]
```

```
Slots:
```

```
Name:  setname  settype  rootfile  filedir  numtrees  treenames
```

```
Class: character character character character  numeric      list
```

```
Known Subclasses:
```

```
Class "SchemeTreeSet", directly
```

```
Class "ProcesSet", directly
```

```
Class "DataTreeSet", by class "ProcesSet", distance 2
```

```
Class "ExprTreeSet", by class "ProcesSet", distance 2
```

```
Class "CallTreeSet", by class "ProcesSet", distance 2
```

```
Class "QualTreeSet", by class "ProcesSet", distance 2
```

```
Class "FilterTreeSet", by class "ProcesSet", distance 2
```

```
Class "AnalysisTreeSet", by class "ProcesSet", distance 2
```

The meaning of the slots is as follows:

**setname:** Object of class "character", representing the name to the ROOT file subdirectory where the ROOT trees are stored, usually one of *DataTreeSet*, *PreprocesSet*, *CallTreeSet*.

**settype:** Object of class "character", describing the type of treeset stored in **setname**, usually one of **scheme**, **rawdata**, **preprocess**.

**rootfile:** Object of class "character", representing the name of the ROOT file, including the full path.

`filedir`: Object of class "character", describing the full path to the system directory where `rootfile` is stored.

`numtrees`: Object of class "numeric", representing the number of ROOT trees stored in subdirectory `setname`.

`treenames`: Object of class "list", representing the names of the ROOT trees stored in subdirectory `setname`.

### 3.2 SchemeTreeSet class

This class extends class `TreeSet` and allows access to the ROOT scheme trees, probe trees and annotation trees. Furthermore, it contains certain array information (slot `probeinfo`) and allows access to the array mask (slot `mask`), describing the probe type.

```
> getClassDef("SchemeTreeSet")
```

```
Class "SchemeTreeSet" [package "xps"]
```

Slots:

```
Name:  chipname  chiptype  probeinfo  probe  unitname  mask
Class: character  character  list data.frame data.frame data.frame
```

```
Name:  setname  settype  rootfile  filedir  numtrees  treenames
Class: character  character  character  character  numeric  list
```

Extends: "TreeSet"

In addition to the slots of `TreeSet` it contains the following slots:

`chipname`: Object of class "character", representing the Affymetrix chip name.

`chiptype`: Object of class "character", representing the chip type, either "GeneChip" or "ExonChip".

`probeinfo`: Object of class "list", representing chip information, including `nrows`, `ncols`, number of probes, etc.

`mask`: Object of class "data.frame". The data.frame can contain the mask used to identify the probes as e.g. PM, MM, or control probes.

As an example, `scheme.test3`, described in Vignette "xps.pdf" contains the information for the Affymetrix 'Test3' expression array:

```
> scheme.test3 <- root.scheme(paste(path.package("xps"), "schemes/SchemeTest3.root", sep="/"))
> str(scheme.test3)
```

```
Formal class 'SchemeTreeSet' [package "xps"] with 12 slots
```

```
..@ chipname : chr "Test3"
..@ chiptype  : chr "GeneChip"
..@ probeinfo: List of 8
.. ..$ nrows   : int 126
.. ..$ ncols   : int 126
.. ..$ nprobes : int 14552
.. ..$ ncontrols : int 13
```

```

.. ..$ ngenes      : int 345
.. ..$ nunits      : int 358
.. ..$ nprobesets: int 358
.. ..$ naffx       : int 0
..@ probe         : 'data.frame':      0 obs. of  0 variables
..@ unitname      : 'data.frame':      0 obs. of  0 variables
..@ mask          : 'data.frame':      0 obs. of  0 variables
..@ setname       : chr "Test3"
..@ settype       : chr "scheme"
..@ rootfile      : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/schemes/SchemeTest3.root"
..@ filedir       : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/schemes"
..@ numtrees      : int 4
..@ treenames:List of 4
.. ..$ : chr "Test3.idx"
.. ..$ : chr "Test3.scm"
.. ..$ : chr "Test3.prb"
.. ..$ : chr "Test3.ann"

```

As this example demonstrates, the ROOT scheme file contains 4 ROOT trees, storing all necessary GeneChip information, including the annotation. All trees can be exported as tables, and optionally also imported as `data.frame`.

The 'Unit' tree with extension *idx* contains information about the processing units, i.e. the Affymetrix probesets, such as an internal 'UNIT\_ID', probeset names and number of cells:

```

> idx <- export(scheme.test3, treetype="idx", outfile="Test3_idx.txt", as.dataframe=TRUE, verbose=FALSE)
> idx[10:16,]

```

|    | UNIT_ID | UnitName         | NumCells | NumAtoms | UnitType |
|----|---------|------------------|----------|----------|----------|
| 10 | -4      | QC10             | 161      | 1        | -5       |
| 11 | -3      | QC11             | 128      | 1        | -12      |
| 12 | -2      | QC12             | 128      | 1        | -11      |
| 13 | -1      | QC13             | 9        | 1        | -13      |
| 14 | 0       | Pae_16SrRNA_s_at | 32       | 16       | 3        |
| 15 | 1       | Pae_23SrRNA_s_at | 32       | 16       | 3        |
| 16 | 2       | PA1178_oprH_at   | 24       | 12       | 3        |

The 'Scheme' tree with extension *scm* provides the chip layout for the different probesets, i.e. the (x,y)-coordinates for each probeset with a defined 'UNIT\_ID':

```

> scm <- export(scheme.test3, treetype="scm", outfile="Test3_scm.txt", as.dataframe=TRUE, verbose=FALSE)
> scm[1843:1848,]

```

|      | UNIT_ID | X   | Y  | ProbeLength | Mask | Atom | ProbeBase | TargetBase |
|------|---------|-----|----|-------------|------|------|-----------|------------|
| 1843 | -1      | 62  | 63 | 25          | -1   | 0    | N         | N          |
| 1844 | -1      | 62  | 64 | 25          | -1   | 0    | N         | N          |
| 1845 | 0       | 111 | 80 | 25          | 0    | 0    | A         | A          |
| 1846 | 0       | 111 | 79 | 25          | 1    | 0    | T         | A          |
| 1847 | 0       | 19  | 19 | 25          | 1    | 1    | A         | T          |
| 1848 | 0       | 19  | 20 | 25          | 0    | 1    | T         | T          |

As shown, this tree contains also a column (leaf) 'Mask', which assigns the probe type to each probe on the array. For expression arrays, probe types are PM with `msk=1`, MM with `msk=0`, and control probes with `msk=-1`. 'Mask' for exon arrays will be described elsewhere.

As default, slot `mask` is empty to save memory (especially when using exon arrays). It is easy to add the 'Mask' to slot `mask` (and remove it, too):

```
> scheme.test3 <- attachMask(scheme.test3)
> msk <- chipMask(scheme.test3)
> scheme.test3 <- removeMask(scheme.test3)
> msk[1843:1848,]
```

| UNIT_ID | X  | Y      | Mask |
|---------|----|--------|------|
| 1843    | -1 | 62 63  | -1   |
| 1844    | -1 | 62 64  | -1   |
| 1845    | 0  | 111 80 | 0    |
| 1846    | 0  | 111 79 | 1    |
| 1847    | 0  | 19 19  | 1    |
| 1848    | 0  | 19 20  | 0    |

The 'Probe' tree with extension `prb` contains the nucleotide sequence for each PM oligonucleotide, as well as the GC-content and the calculated melting temperature `Tm`:

```
> prb <- export(scheme.test3, treetype="prb", outfile="Test3_prb.txt", as.dataframe=TRUE, verbose=FALSE)
> prb[1843:1848,]
```

| ProbeSetID | ProbeX | ProbeY | ProbeInterrogationPosition |
|------------|--------|--------|----------------------------|
| 1843       | -1     | 62     | 63                         |
| 1844       | -1     | 62     | 64                         |
| 1845       | 0      | 111    | 80                         |
| 1846       | 0      | 111    | 79                         |
| 1847       | 0      | 19     | 19                         |
| 1848       | 0      | 19     | 20                         |

  

| ProbeSetID | ProbeSequence             | ContentGC | Tm | ProbeType |
|------------|---------------------------|-----------|----|-----------|
| 1843       | N                         | -1        | -1 | -1        |
| 1844       | N                         | -1        | -1 | -1        |
| 1845       | N                         | 14        | 73 | 1         |
| 1846       | TGCCTAGGAATCTGCCTGGTAGTGG | 14        | 73 | 1         |
| 1847       | CGCTAATACCGCATACGTCCTGAGG | 14        | 73 | 1         |
| 1848       | N                         | 14        | 73 | 1         |

Finally, the transcript 'Annotation' tree with extension `ann` contains the probeset annotation, such as gene name and symbol:

```
> ann <- export(scheme.test3, treetype="ann", outfile="Test3_ann.txt", as.dataframe=TRUE, verbose=FALSE)
> head(ann)
```

| UNIT_ID | ProbesetID         |
|---------|--------------------|
| 1       | 0 Pae_16SrRNA_s_at |
| 2       | 1 Pae_23SrRNA_s_at |
| 3       | 2 PA1178_oprH_at   |
| 4       | 3 PA1816_dnaQ_at   |
| 5       | 4 PA3183_zwf_at    |
| 6       | 5 PA3640_dnaE_at   |

| UNIT_ID | GeneName | GeneSymbol |
|---------|----------|------------|
| 1       | <NA>     | <NA>       |
| 2       | <NA>     | <NA>       |

```

3 PhoP/Q and low Mg2+ inducible outer membrane protein H1 precursor      oprH
4                               DNA polymerase III, epsilon chain        dnaQ
5                               glucose-6-phosphate 1-dehydrogenase      zwf
6                               DNA polymerase III, alpha chain          dnaE
  GeneAccession  EntrezID  Chromosome  Cytoband  Start  Stop  Strand
1             <NA>      -1         NA      <NA>   -1   -1     ?
2             <NA>      -1         NA      <NA>   -1   -1     ?
3             <NA>      -1         NA      <NA>   -1   -1     ?
4             <NA>      -1         NA      <NA>   -1   -1     ?
5             <NA>      -1         NA      <NA>   -1   -1     ?
6             <NA>      -1         NA      <NA>   -1   -1     ?

```

The ROOT *scheme* files for exon arrays contain additional tree types, see the help file `?validTreeType`.

### 3.3 ProceSet class

This is the common base class for subclasses *DataTreeSet*, *ExprTreeSet*, *CallTreeSet* and *QualTreeSet*, respectively, and contains the following slots:

```
> getClassDef("ProceSet")
```

```
Class "ProceSet" [package "xps"]
```

```
Slots:
```

```
Name:      scheme      data      params      setname      settype
Class: SchemeTreeSet  data.frame  list      character    character
```

```
Name:      rootfile    filedir    numtrees    treenames
Class:     character    character  numeric     list
```

```
Extends: "TreeSet"
```

```
Known Subclasses: "DataTreeSet", "ExprTreeSet", "CallTreeSet", "QualTreeSet", "FilterTreeSet",
"AnalysisTreeSet"
```

The additional slots are:

**scheme:** Object of class "SchemeTreeSet", providing access to the ROOT scheme file.

**data:** Object of class "data.frame". The data.frame can contain the data stored in ROOT data trees.

**params:** Object of class "list" representing relevant parameters.

The content of slot **data** depends on the type of subclass:

For subclass *DataTreeSet* slot **data** is reserved for the probe data, however, it is empty by default to avoid potential memory problems with large datasets. For subclasses *ExprTreeSet* and *CallTreeSet* slot **data** contains expression levels and detection p-values, respectively.

### 3.4 DataTreeSet class

Class *DataTreeSet* is usually created when importing raw CEL-files as ROOT trees into a ROOT data file, or accessing an existing ROOT data file, using functions `import.data` or `root.data`, respectively. However, certain preprocessing functions such as `bgcorrect` can also result in the creation of class *DataTreeSet*. The slots are:

```
> getClassDef("DataTreeSet")
```

```
Class "DataTreeSet" [package "xps"]
```

```
Slots:
```

```
Name:    bgtreenames      bgrd    projectinfo      scheme      data
Class:    list           data.frame ProjectInfo SchemeTreeSet data.frame
```

```
Name:    params          setname    settype    rootfile    filedir
Class:    list           character  character  character    character
```

```
Name:    numtrees      treenames
Class:    numeric      list
```

```
Extends:
```

```
Class "ProcesSet", directly
```

```
Class "TreeSet", by class "ProcesSet", distance 2
```

Following additional slots are defined for class *DataTreeSet*:

**bgtreenames**: Object of class "list", representing the names of optional ROOT background trees.

**bgrd**: Object of class "data.frame". The data.frame can contain background intensities stored in ROOT background trees.

**projectinfo**: Object of class "ProjectInfo", containing information about the project.

Slots **bgtreenames** and **bgrd** are reserved for optional background tree names and data, respectively.

Slot **projectinfo** allows to save optional project information defined in class *ProjectInfo* described below. The project information will not only be stored in class *DataTreeSet*, but also in the ROOT data file containing the raw data from the CEL-files, when using functions `import.data` or `addData`, respectively.

As an example, `data.test3`, described in Vignette "xps.pdf" contains the information to access the CEL-files from the 'Test3' expression array, which are stored as ROOT trees in ROOT data file *DataTest3\_cel.root*:

```
> data.test3 <- root.data(scheme.test3, paste(path.package("xps"), "rootdata/DataTest3_cel.root", sep="/")
> str(data.test3)
```

```
Formal class 'DataTreeSet' [package "xps"] with 12 slots
```

```
..@ bgtreenames: list()
```

```
..@ bgrd      :'data.frame':      0 obs. of  0 variables
```

```
..@ projectinfo:Formal class 'ProjectInfo' [package "xps"] with 15 slots
```

```
.. .. ..@ submitter      : chr ""
```

```
.. .. ..@ laboratory     : chr ""
```

```
.. .. ..@ contact       : chr ""
```

```
.. .. ..@ project       : list()
```

```
.. .. ..@ author        : list()
```

```
.. .. ..@ dataset       : list()
```

```
.. .. ..@ source        : list()
```

```
.. .. ..@ sample        : list()
```

```
.. .. ..@ celline       : list()
```



```

.. .. ..@ primarycell   : list()
.. .. ..@ tissue       : list()
.. .. ..@ biopsy       : list()
.. .. ..@ arraytype    : list()
.. .. ..@ hybridizations:'data.frame':      0 obs. of  0 variables
.. .. ..@ treatments   :'data.frame':      0 obs. of  0 variables
..@ scheme             :Formal class 'SchemeTreeSet' [package "xps"] with 12 slots
.. .. ..@ chipname     : chr "Test3"
.. .. ..@ chiptype     : chr "GeneChip"
.. .. ..@ probeinfo:List of 8
.. .. .. ..$ nrows      : int 126
.. .. .. ..$ ncols      : int 126
.. .. .. ..$ nprobes    : int 14552
.. .. .. ..$ ncontrols  : int 13
.. .. .. ..$ ngenes     : int 345
.. .. .. ..$ nunits     : int 358
.. .. .. ..$ nprobesets: int 358
.. .. .. ..$ naffx      : int 0
.. .. ..@ probe       :'data.frame':      0 obs. of  0 variables
.. .. ..@ unitname    :'data.frame':      0 obs. of  0 variables
.. .. ..@ mask        :'data.frame':      0 obs. of  0 variables
.. .. ..@ setname     : chr "Test3"
.. .. ..@ settype     : chr "scheme"
.. .. ..@ rootfile    : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/schemes/SchemeTest3.root"
.. .. ..@ filedir     : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/schemes"
.. .. ..@ numtrees    : int 4
.. .. ..@ treenames:List of 4
.. .. .. ..$ : chr "Test3.idx"
.. .. .. ..$ : chr "Test3.scm"
.. .. .. ..$ : chr "Test3.prb"
.. .. .. ..$ : chr "Test3.ann"
..@ data              :'data.frame':      0 obs. of  0 variables
..@ params            : list()
..@ setname           : chr "DataSet"
..@ settype           : chr "rawdata"
..@ rootfile          : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/rootdata/DataTest3_cel.root"
..@ filedir           : chr "/tmp/RtmpC0QXP6/Rinst31c552d200e0/xps/rootdata"
..@ numtrees          : int 4
..@ treenames         :List of 4
.. ..$ : chr "TestA1.cel"
.. ..$ : chr "TestA2.cel"
.. ..$ : chr "TestB1.cel"
.. ..$ : chr "TestB2.cel"

```

As mentioned, slot `data` is initially empty to avoid memory problems with large datasets, especially exon array datasets. Functions `attachInten` and `removeInten` allow to attach/remove these data, respectively, as described in Vignette "xps.pdf".

### 3.5 ExprTreeSet class

Class *ExprTreeSet* is obtained as result of preprocessing the raw data, i.e. summarization, or as result of normalizing preprocessed data, respectively. It contains the expression levels in slot `data`. It has the

following slots:

```
> getClassDef("ExprTreeSet")
```

```
Class "ExprTreeSet" [package "xps"]
```

```
Slots:
```

|        |           |           |               |            |        |
|--------|-----------|-----------|---------------|------------|--------|
| Name:  | exprtype  | normtype  | scheme        | data       | params |
| Class: | character | character | SchemeTreeSet | data.frame | list   |

|        |           |           |           |           |          |
|--------|-----------|-----------|-----------|-----------|----------|
| Name:  | setname   | settype   | rootfile  | filedir   | numtrees |
| Class: | character | character | character | character | numeric  |

|        |           |
|--------|-----------|
| Name:  | treenames |
| Class: | list      |

```
Extends:
```

```
Class "ProcesSet", directly
```

```
Class "TreeSet", by class "ProcesSet", distance 2
```

The additional slots are:

exprtype: Object of class "character", representing the expression type, i.e. rma, mas5, mas4 or custom.

normtype: Object of class "character", representing the normalization type, i.e. none, mean, median, lowess,supsmu.

### 3.6 CallTreeSet class

Class *CallTreeSet* allows to access the Affymetrix detection calls and corresponding p-values, either the MAS5 detection calls or the detection above background (DABG) calls. It is obtained as result of functions `mas5.call` or `dabg.call`, respectively. It has the following slots:

```
> getClassDef("CallTreeSet")
```

```
Class "CallTreeSet" [package "xps"]
```

```
Slots:
```

|        |           |            |               |            |        |
|--------|-----------|------------|---------------|------------|--------|
| Name:  | calltype  | detcall    | scheme        | data       | params |
| Class: | character | data.frame | SchemeTreeSet | data.frame | list   |

|        |           |           |           |           |          |
|--------|-----------|-----------|-----------|-----------|----------|
| Name:  | setname   | settype   | rootfile  | filedir   | numtrees |
| Class: | character | character | character | character | numeric  |

|        |           |
|--------|-----------|
| Name:  | treenames |
| Class: | list      |

```
Extends:
```

```
Class "ProcesSet", directly
```

```
Class "TreeSet", by class "ProcesSet", distance 2
```

The additional slots are:

`calltype`: Object of class "character", representing the call type, i.e. "mas5" or "dabg".

`detcall`: Object of class "data.frame". The data.frame can contain the detection calls stored in ROOT call trees.

Slot `data` contains the detection call p-values while slot `detcall` contains the detection calls.

### 3.7 QualTreeSet class

Class *QualTreeSet* is obtained as result of fitting probe level models. It has the following slots:

```
> getClassDef("QualTreeSet")
```

```
Class "QualTreeSet" [package "xps"]
```

```
Slots:
```

|        |           |           |               |            |        |
|--------|-----------|-----------|---------------|------------|--------|
| Name:  | qualtype  | qualopt   | scheme        | data       | params |
| Class: | character | character | SchemeTreeSet | data.frame | list   |

|        |           |           |           |           |          |
|--------|-----------|-----------|-----------|-----------|----------|
| Name:  | setname   | settype   | rootfile  | filedir   | numtrees |
| Class: | character | character | character | character | numeric  |

|        |           |
|--------|-----------|
| Name:  | treenames |
| Class: | list      |

```
Extends:
```

```
Class "ProcesSet", directly
```

```
Class "TreeSet", by class "ProcesSet", distance 2
```

The additional slots are:

`qualtype`: Object of class "character", representing the quality control option, i.e. 'raw', 'adjusted', 'normalized' or 'all'.

`qualopt`: Object of class "character", representing the quality control type, i.e. 'rlm' the normalization.

### 3.8 ProjectInfo class

This class is a stand-alone supporting S4 class and allows to store phenotypic and MIAME-like project information. It contains the following slots:

```
> getClassDef("ProjectInfo")
```

```
Class "ProjectInfo" [package "xps"]
```

```
Slots:
```

|        |           |            |           |         |
|--------|-----------|------------|-----------|---------|
| Name:  | submitter | laboratory | contact   | project |
| Class: | character | character  | character | list    |

|        |        |         |        |        |
|--------|--------|---------|--------|--------|
| Name:  | author | dataset | source | sample |
| Class: | list   | list    | list   | list   |

|        |         |             |        |        |
|--------|---------|-------------|--------|--------|
| Name:  | celline | primarycell | tissue | biopsy |
| Class: | list    | list        | list   | list   |

|        |           |                |            |
|--------|-----------|----------------|------------|
| Name:  | arraytype | hybridizations | treatments |
| Class: | list      | data.frame     | data.frame |

submitter: Object of class "character", representing the name of the submitter.

laboratory: Object of class "character", representing the laboratory of the submitter.

contact: Object of class "character", representing the contact address of the submitter.

project: Object of class "list", representing the project information.

author: Object of class "list", representing the author information.

dataset: Object of class "list", representing the dataset information.

source: Object of class "list", representing the sample source information.

sample: Object of class "list", representing the sample information.

celline: Object of class "list", representing the sample information for cell lines.

primarycell: Object of class "list", representing the sample information for primary cells.

tissue: Object of class "list", representing the sample information for tissues.

biopsy: Object of class "list", representing the sample information for biopsies.

arraytype: Object of class "list", representing the array information.

hybridizations: Object of class "data.frame", representing the hybridization information for each hybridization.

treatments: Object of class "data.frame", representing the treatment information for each hybridization.

This class must be created explicitly first using the constructor function `ProjectInfo`, before it can be added to class `DataTreeSet`. Here is a simple example for `data.test3`:

```
> project <- ProjectInfo(submitter="Christian", laboratory="home",contact="email")
> projectInfo(project) <- c("TestProject","20060106","Project Type","use Test3 data for testing","m
> authorInfo(project) <- c("Stratowa","Christian","Project Leader","Company","Dept","cstrato.at.ao
> datasetInfo(project) <- c("Test3Set","MC","Tissue","Stratowa","20060106","description","my commen
> sourceInfo(project) <- c("Unknown","source type","Homo sapiens","caucasian","description","my co
> primcellInfo(project) <- c("Mel131","primary cell",20071123,"extracted from patient","male","my phe
> arrayInfo(project) <- c("Test3","GeneChip","description","my comment")
> hybridizInfo(project) <- c(c("TestA1","hyb type","TestA1.CEL",20071117,"my prep1","standard protoc
+ c("TestA2","hyb type","TestA2.CEL",20071117,"my prep2","standard protoc
+ c("TestB1","hyb type","TestB1.CEL",20071117,"my prep1","standard protoc
+ c("TestB2","hyb type","TestB2.CEL",20071117,"my prep2","standard protoc
> treatmentInfo(project) <- c(c("TestA1","DMSO",4.3,"mM",1.0,"hours","intravenous","my comment"),
+ c("TestA2","DMSO",4.3,"mM",8.0,"hours","intravenous","my comment"),
+ c("TestB1","DrugA2",4.3,"mM",1.0,"hours","intravenous","my comment"),
+ c("TestB2","DrugA2",4.3,"mM",8.0,"hours","intravenous","my comment"))
> show(project)
```

Project information:

Submitter: Christian

Laboratory: home

Contact: email

Information is available on: project, author, dataset, source, sample, primarycell, arraytype, hybrid

### 3.9 Filter class

This is the base class for the S4 classes *PreFilter* and *UniFilter*.

```
> getClassDef("Filter")
```

```
Class "Filter" [package "xps"]
```

```
Slots:
```

```
Name: numfilters
```

```
Class: numeric
```

```
Known Subclasses: "PreFilter", "UniFilter"
```

The meaning of the slots is as follows:

`numfilters`: Object of class "numeric" giving the number of filters applied.

### 3.10 PreFilter class

Class *PreFilter* allows to apply different filters to class *ExprTreeSet*, i.e. to the expression level data.frame data..

```
> getClassDef("PreFilter")
```

```
Class "PreFilter" [package "xps"]
```

```
Slots:
```

```
Name:      mad      cv      variance  difference      ratio      gap
Class:     list     list     list      list          list      list
```

```
Name: lothreshold hithreshold  quantile  prescall  numfilters
Class: list       list       list      list      list      numeric
```

```
Extends: "Filter"
```

The meaning of the slots is as follows:

`mad`: Object of class "list" describing parameters for `madFilter`.

`cv`: Object of class "list" describing parameters for `cvFilter`.

`variance`: Object of class "list" describing parameters for `varFilter`.

`difference`: Object of class "list" describing parameters for `diffFilter`.

`ratio`: Object of class "list" describing parameters for `RratioFilter`.

gap:Object of class "list" describing parameters for RgapFilter.

hithreshold:Object of class "list" describing parameters for highFilter.

lothreshold:Object of class "list" describing parameters for lowFilter.

quantile:Object of class "list" describing parameters for quantileFilter.

prescall:Object of class "list" describing parameters for callFilter.

This class must be created explicitly using the constructor function `PreFilter`, and is added as parameter `filter` to function `prefilter`. Here is an example, where all filters are initialized for demonstration purposes only:

```
> prefltr <- PreFilter()
> madFilter(prefltr) <- c(0.5,0.01)
> cvFilter(prefltr) <- c(0.3,0.0,0.01)
> varFilter(prefltr) <- c(0.6,0.02,0.01)
> diffFilter(prefltr) <- c(2.2,0.0,0.01)
> ratioFilter(prefltr) <- c(1.5)
> gapFilter(prefltr) <- c(0.3,0.05,0.0,0.01)
> lowFilter(prefltr) <- c(4.0,3,"samples")
> highFilter(prefltr) <- c(14.5,75.0,"percent")
> quantileFilter(prefltr) <- c(3.0, 0.05, 0.95)
> callFilter(prefltr) <- c(0.02,80.0,"percent")
> str(prefltr)
```

Formal class 'PreFilter' [package "xps"] with 11 slots

```
..@ mad      :List of 2
.. ..$ cutoff : num 0.5
.. ..$ epsilon: num 0.01
..@ cv       :List of 3
.. ..$ cutoff : num 0.3
.. ..$ trim   : num 0
.. ..$ epsilon: num 0.01
..@ variance :List of 3
.. ..$ cutoff : num 0.6
.. ..$ trim   : num 0.02
.. ..$ epsilon: num 0.01
..@ difference :List of 3
.. ..$ cutoff : num 2.2
.. ..$ trim   : num 0
.. ..$ epsilon: num 0.01
..@ ratio     :List of 1
.. ..$ cutoff: num 1.5
..@ gap       :List of 4
.. ..$ cutoff : num 0.3
.. ..$ window : num 0.05
.. ..$ trim   : num 0
.. ..$ epsilon: num 0.01
..@ lothreshold:List of 3
.. ..$ cutoff : num 4
.. ..$ parameter: num 3
```

```

.. ..$ condition: chr "samples"
..@ hithreshold:List of 3
.. ..$ cutoff : num 14.5
.. ..$ parameter: num 75
.. ..$ condition: chr "percent"
..@ quantile :List of 3
.. ..$ cutoff : num 3
.. ..$ loquantile: num 0.05
.. ..$ hiquantile: num 0.95
..@ prescall :List of 3
.. ..$ cutoff : num 0.02
.. ..$ samples : num 80
.. ..$ condition: chr "percent"
..@ numfilters : num 10

```

### 3.11 UniFilter class

Class *UniFilter* allows to apply different unitest filters to class *ExprTreeSet*, i.e. to the expression level data.frame data.

```
> getClassDef("UniFilter")
```

```
Class "UniFilter" [package "xps"]
```

Slots:

```
Name: foldchange  prescall  unifilter  unitest  numfilters
Class:      list      list      list      list      numeric
```

```
Extends: "Filter"
```

The meaning of the slots is as follows:

*foldchange*: Object of class "list" describing parameters for *fcFilter*.

*prescall*: Object of class "list" describing parameters for *callFilter*.

*unifilter*: Object of class "list" describing parameters for *unitestFilter*.

*unitest*: Object of class "list" describing parameters for *uniTest*.

This class must be created explicitly using the constructor function *UniFilter*, and is added as parameter *filter* to function *unifilter*. Here is an example, where all filters are initialized for demonstration purposes only:

```

> unifltr <- UniFilter()
> fcFilter(unifltr) <- c(1.5, "both")
> callFilter(unifltr) <- c(0.02, 80.0, "percent")
> unitestFilter(unifltr) <- c(0.01, "pval")
> uniTest(unifltr) <- c("t.test", "two.sided", "wy", 5000, 0.0, FALSE, 0.98, TRUE)
> str(unifltr)

```

```
Formal class 'UniFilter' [package "xps"] with 5 slots
```

```
..@ foldchange:List of 2
```

```

.. ..$ cutoff      : num 1.5
.. ..$ direction:  chr "both"
..@ prescall      :List of 3
.. ..$ cutoff      : num 0.02
.. ..$ samples     : num 80
.. ..$ condition:  chr "percent"
..@ unifilter     :List of 2
.. ..$ cutoff      : num 0.01
.. ..$ variable:   chr "pval"
..@ unitest       :List of 8
.. ..$ type        : chr "t.test"
.. ..$ alternative: chr "two.sided"
.. ..$ correction : chr "wy"
.. ..$ numperm     : int 5000
.. ..$ mu          : num 0
.. ..$ paired      : logi FALSE
.. ..$ conflevel   : num 0.98
.. ..$ varequ      : logi TRUE
..@ numfilters:   num 2

```

### 3.12 FilterTreeSet class

Class *FilterTreeSet* is obtained as result of filtering an instance of class *ExprTreeSet*. It contains the filter mask in slot *data*.

```
> getClassDef("FilterTreeSet")
```

```
Class "FilterTreeSet" [package "xps"]
```

Slots:

|        |          |             |             |               |            |
|--------|----------|-------------|-------------|---------------|------------|
| Name:  | filter   | exprset     | callset     | scheme        | data       |
| Class: | Filter   | ExprTreeSet | CallTreeSet | SchemeTreeSet | data.frame |
| Name:  | params   | setname     | settype     | rootfile      | filedir    |
| Class: | list     | character   | character   | character     | character  |
| Name:  | numtrees | treenames   |             |               |            |
| Class: | numeric  | list        |             |               |            |

Extends:

Class "ProcesSet", directly

Class "TreeSet", by class "ProcesSet", distance 2

In addition to the slots of classes *ProcesSet* and *TreeSet* it contains the following slots:

*filter*: Object of class "Filter" currently providing access to the *PreFilter* settings.

*exprset*: Object of class "ExprTreeSet" providing direct access to the *ExprTreeSet* used for filtering.

*callset*: Object of class "CallTreeSet" providing direct access to the optional *CallTreeSet* used for filtering.



### 3.13 AnalysisTreeSet class

Class *AnalysisTreeSet* is obtained as result of filtering an instance of class *ExprTreeSet* using function `unifilter`. It contains currently the results of the univariate analysis in slot `data`.

```
> getClassDef("AnalysisTreeSet")
```

```
Class "AnalysisTreeSet" [package "xps"]
```

```
Slots:
```

|        |               |               |            |          |           |
|--------|---------------|---------------|------------|----------|-----------|
| Name:  | fltrset       | scheme        | data       | params   | setname   |
| Class: | FilterTreeSet | SchemeTreeSet | data.frame | list     | character |
| Name:  | settype       | rootfile      | filedir    | numtrees | treenames |
| Class: | character     | character     | character  | numeric  | list      |

```
Extends:
```

```
Class "ProcesSet", directly
```

```
Class "TreeSet", by class "ProcesSet", distance 2
```

In addition to the slots of classes *ProcesSet* and *TreeSet* it contains the following slots:

`fltrset`: Object of class "FilterTreeSet" providing indirect access to the *ExprTreeSet* used and the *UniFilter* settings.

## References

The ROOT team. ROOT User Guide. Technical report, CERN, 2009. URL <http://root.cern.ch/drupal/content/users-guide>.