

the *biocViews* package

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1 Overview

Bioconductor is a project supporting statistical computations and inference in high-throughput biological experimentation. Currently the project consists of containers, workflow components, and multiscale documentation useful in the areas of

- DNA microarray preprocessing and analysis,
- array CGH, SAGE, proteomic, and cell-based assay preprocessing and analysis,
- annotation of experimental processes and results,
- graph and network structures relevant to bioinformatics.

Bioconductor software is currently organized into over 100 R packages. R packages are collections of folders populated with program code in R and other languages, compiled datasets used for annotation or software demonstration, and documentation.

The use of R packages use of packages is helpful to both users and developers. At the user level, R provides high-level processes for installing R packages with checksum verification, and for presenting/executing documentation at the package or package-component level. At the developer level, R provides high-level processes for carrying out package quality control, including verifying the structure of the package, the coverage of supplied documentation, and the freedom from error of various example computations supplied in the documentation sources.

Large collections of R packages are difficult to survey without special guidance. This document describes how a task view vocabulary can be constructed and used to provide a hypertext interface to a catalog of R packages. Section 5 below gives a concise step-by-step summary of the activities required.

2 A vocabulary graph and some manipulations

A possible vocabulary for bioconductor package topics has been created as a directed graph, saved as `bcVoc` in the *biocViews* package.

```
> data(bcVoc)
> bcVoc
```

A graphNEL graph with directed edges

Number of Nodes = 68

Number of Edges = 68

This graph was created with the graphviz dot language, then converted to GXL using graphviz dot2gxl utility, then imported to R using `graph::fromGXL`. To see the top-level terms of the vocabulary, use

```
> adj(bcVoc, "vocRoot")
```

```
$vocRoot
```

```
[1] "ArrayCGH"
[2] "FlowCytometry"
[3] "Proteomics"
[4] "DNAMicroarrayPreprocessing"
[5] "StatisticalModelingForHighThroughputBiology"
[6] "GraphsAndNetworks"
[7] "Visualization"
[8] "Ontologies"
[9] "SequenceAnalysis"
```

```
[10] "Databases"
[11] "QuantitativeGenetics"
[12] "Annotation"
[13] "GeneralInfrastructure"
[14] "biocMiscellaneous"
[15] "SAGE"
```

To see all concept terms subordinate to “ontologies”, use

```
> acc(bcVoc, "Ontologies")
```

```
$Ontologies
      otherOntology OntologyInfrastructure      MAGEasOntology
                1                      1                      1
      GOasOntology
                1
```

The entire term set is listed in the appendix.

3 Associating packages with vocabulary terms

The `packAssoc` function will associate each element of a vector of package names with (at present) a single term in the vocabulary. This works using a trivial GUI. The R interpreter prompts the user to give top level, second level (if relevant given top level), and third level (if relevant given second level) terms associated with each package named in the `packlist` argument. The vocabulary graph is given as the second argument.

Suppose our package list is

```
> demop <- c("Biobase", "graph", "limma", "factDesign")
```

Then

```
> pal <- packAssoc(demop, bcVoc)
```

loads `pal` with a list, after the GUI has been used.

```
> names(pal)
```

```
[1] "Biobase"      "graph"        "limma"        "factDesign"
```

```
> pal$factDesign
```

```

$top
[1] "StatisticalModelingForHighThroughputBiology"

$second
[1] "DifferentialExpression"

$third
[1] "FactorialDesign"

$maintainer
[1] "Denise Scholtens <dscholte@hsph.harvard.edu>"

$packagename
[1] "factDesign"

$desc
[1] "This package provides a set of tools for analyzing data from a factorial designed

$title
[1] "Factorial designed microarray experiment analysis"

Some of the information saved is derived from calls to packageDescription.
The package:terminology associations can be permuted:

> vpal <- packAssoc2viewlist(pal)
> vpal

$DifferentialExpression
[1] "limma"      "factDesign"

$FactorialDesign
[1] "factDesign"

$GeneralInfrastructure
[1] "Biobase"

$GraphInfrastructure
[1] "graph"

$GraphsAndNetworks
[1] "graph"

$LinearModels

```

```
[1] "limma"
```

```
$StatisticalModelingForHighThroughputBiology
```

```
[1] "limma"      "factDesign"
```

This enables us to build *ctv* structures.

4 Building *ctv* documents

ctv documents are XML markups of view-related metadata. The appendix includes a full example of a *ctv* view document.

The basic structural elements are currently:

- `<CRANTaskView>` is the root tag
- `<name>`, `<topic>`, `<maintainer>`; self-explanatory except for `topic`, which is a plaintext rendering of the topic; the maintainer must also be plaintext, apparently owing to XML syntax restrictions
- `<info>`; can hold a rich HTML markup of narrative about the view, including references to packages, which are marked up with `<pkg>`
- `<packagelist>`, a list of packages marked up with `<pkg>`
- `<links>`, a list of URLs marked up as pure HTML anchors

The `makeCTV` function helps to create such a document from the elements of a view-package-vocabulary association list created by `packAssoc2vlist`. A trivial illustration:

```
> vn <- names(vpal)
> c1 <- makeCTV(vn[1], vn[1], "None", vpal[[1]], "None", bcVoc)
```

Loading required package: XML

```
> targ <- tempfile()
> saveXML(c1, file = targ)
> dem <- read.ctv(targ)
> dem
```

CRAN Task View

```
Name:      DifferentialExpression
Topic:     DifferentialExpression
Maintainer: None
```

```
Packages:  factDesign, limma
```

To run this over our entire view set, we can use:

```
> allc <- getCTVs(vpal, bcVoc)
```

I now have a list of CTV structures in R. We'll serialize them to HTML:

```
> jnk <- sapply(allc, ctv2html)
```

In addition to the view-specific HTML pages, we need a top-level entry point. The `topwrap` function helps with this.

```
> els <- topwrap(bcVoc)
> toptop <- readLines(system.file("htmlfrags/topfrag.html", package = "biocViews"))
> cat(toptop, els, "</ul>\n")
```

```
<html> <head>   <title>Bioconductor Task View: top level views</title>   <link rel=styl
<li><a href=FlowCytometry.html>FlowCytometry</a>
<li><a href=Proteomics.html>Proteomics</a>
<li><a href=DNAMicroarrayPreprocessing.html>DNAMicroarrayPreprocessing</a>
<ul><li> subviews: <a href=cDNAPreproc.html>cDNAPreproc</a>, <a href=AffyPreproc.html>
<li><a href=StatisticalModelingForHighThroughputBiology.html>StatisticalModelingForHig
<ul><li> subviews: <a href=ClusterAnalysis.html>ClusterAnalysis</a>, <a href=Functiona
<li><a href=GraphsAndNetworks.html>GraphsAndNetworks</a>
<ul><li> subviews: <a href=GraphInfrastructure.html>GraphInfrastructure</a>, <a href=G
<li><a href=Visualization.html>Visualization</a>
<ul><li> subviews: <a href=VisualizationInfrastructure.html>VisualizationInfrastructur
<li><a href=Ontologies.html>Ontologies</a>
<ul><li> subviews: <a href=OntologyInfrastructure.html>OntologyInfrastructure</a>, <a
<li><a href=SequenceAnalysis.html>SequenceAnalysis</a>
<ul><li> subviews: <a href=SequenceSimilarity.html>SequenceSimilarity</a>, <a href=Seq
<li><a href=Databases.html>Databases</a>
<ul><li> subviews: <a href=DatabaseInfrastructure.html>DatabaseInfrastructure</a>, <a
<li><a href=QuantitativeGenetics.html>QuantitativeGenetics</a>
<li><a href=Annotation.html>Annotation</a>
<ul><li> subviews: <a href=AnnotationInfrastructure.html>AnnotationInfrastructure</a>,
<li><a href=GeneralInfrastructure.html>GeneralInfrastructure</a>
<li><a href=biocMiscellaneous.html>biocMiscellaneous</a>
<li><a href=SAGE.html>SAGE</a>
</ul>
```

The resulting HTML can be installed as `index.html` in the directory holding all the other view files emitted by the application of `ctv2html` shown above.

Figures 1 and 2 illustrate some view-specific outputs.

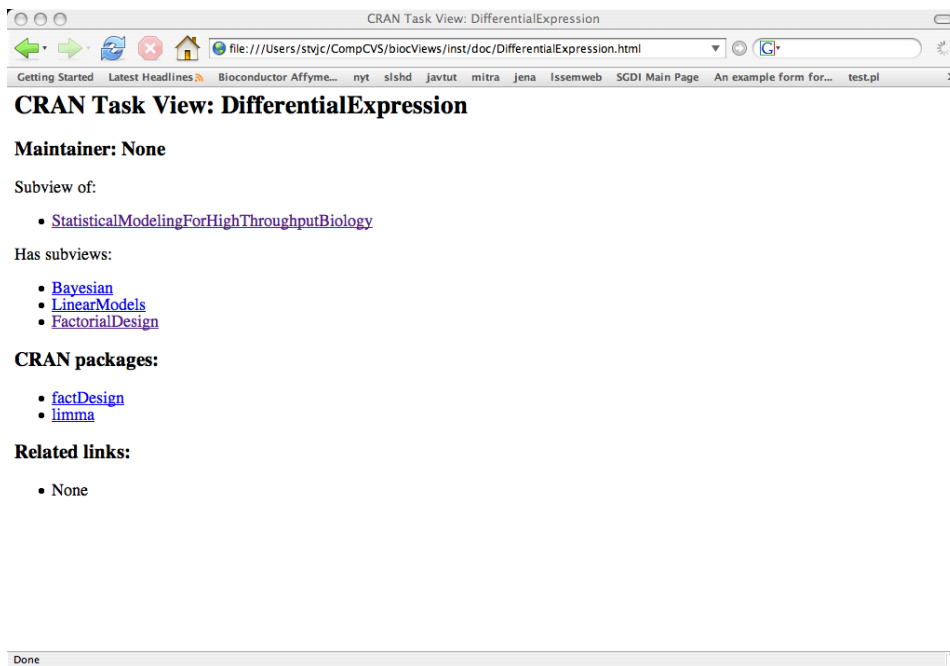


Figure 1: A view of one of the generated HTML pages. To proceed, we need systematic ways of populating the narrative components.

5 Summary of activities

1. Create a vocabulary graph. The dot language can be used very conveniently. Serialize this to GXL using graphviz dot2gxl and then import using R `graph::fromGXL`.
2. Create a package list. A character vector in R of packages that are installed in the image of R to be used for view generation.
3. Create a package-view association structure. This can be very laborious, but is interruptible using `packAssoc`. Permute this structure to a viewlist using `packAssoc2viewlist`.
4. Transform viewlist to ctv structures using `getCTVs`. The ctv structures generated here respect aspects of the vocabulary hierarchy, so the vocabulary graph must be identified as a an argument to `getCTVs`.
5. Create an entry page using `topwrap`. Move the folder including all generated HTML to a web-accessible location.

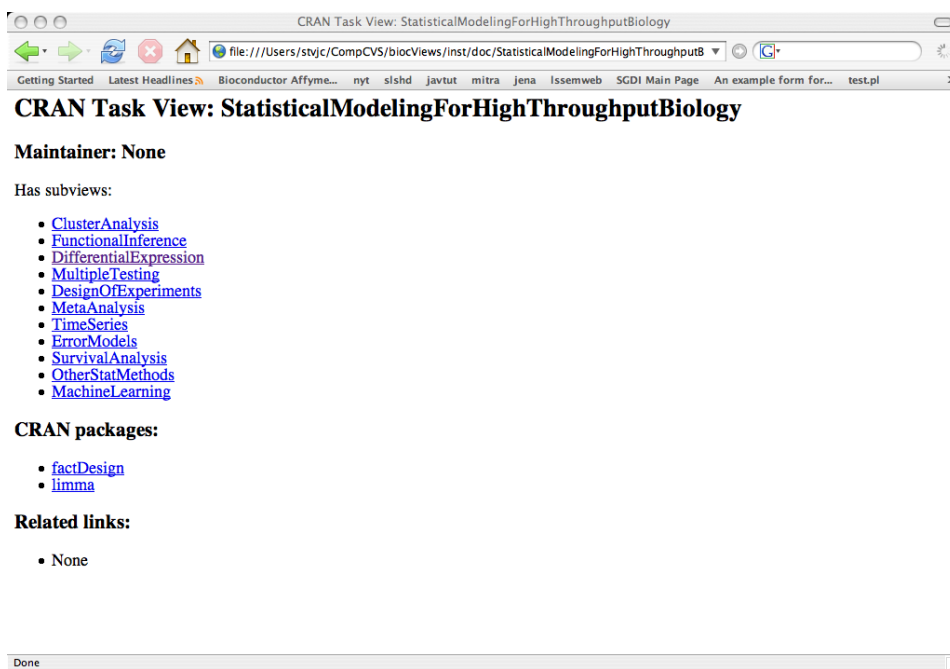


Figure 2: Here's a higher level page on a rich topic set.

6 Appendix

6.1 The full vocabulary

```
> sort(nodes(bcVoc))

[1] "AffyAnnotation"
[2] "AffyPreproc"
[3] "Annotation"
[4] "AnnotationInfrastructure"
[5] "ArrayCGH"
[6] "arrayQC"
[7] "Bayesian"
[8] "biocMiscellaneous"
[9] "cDNAPreproc"
[10] "ChromosomeVisualization"
[11] "ClusterAnalysis"
[12] "DatabaseInfrastructure"
[13] "Databases"
[14] "DesignOfExperiments"
[15] "DifferentialExpression"
[16] "DNAMicroarrayPreprocessing"
[17] "ErrorModels"
[18] "ExternalQueryResolutionWithSequence"
[19] "FactorialDesign"
[20] "FlowCytometry"
[21] "FunctionalInference"
[22] "GeneFiltering"
[23] "GeneralInfrastructure"
[24] "GeneralVisualization"
[25] "GOasOntology"
[26] "GraphDataExamples"
[27] "GraphInfrastructure"
[28] "GraphsAndNetworks"
[29] "GraphVisualization"
[30] "HumanPlatform"
[31] "InferenceOnGraphs"
[32] "LinearModels"
[33] "MachineLearning"
[34] "MAGEasOntology"
[35] "MetaAnalysis"
[36] "MultipleTesting"
[37] "nonHumanPlatform"
```

[38] "Ontologies"
[39] "OntologyInfrastructure"
[40] "OrganismAnnotation"
[41] "otherAffypp"
[42] "othercDNApp"
[43] "OtherDesign"
[44] "OtherDiffExp"
[45] "OtherFunc"
[46] "otherOntology"
[47] "OtherPreproc"
[48] "otherSeqDB"
[49] "OtherStatMethods"
[50] "PlatformAnnotation"
[51] "ProbeLevelModels"
[52] "ProbeMatching"
[53] "Proteomics"
[54] "QuantitativeGenetics"
[55] "SAGE"
[56] "SampleSize"
[57] "SequenceAnalysis"
[58] "SequenceDatabases"
[59] "SequenceInfrastructure"
[60] "SequenceSimilarity"
[61] "StatisticalModelingForHighThroughputBiology"
[62] "SurvivalAnalysis"
[63] "TimeSeries"
[64] "Visualization"
[65] "VisualizationInfrastructure"
[66] "vocRoot"
[67] "WithGO"
[68] "WithPubMed"

6.2 Snapshots of vocabulary subgraphs

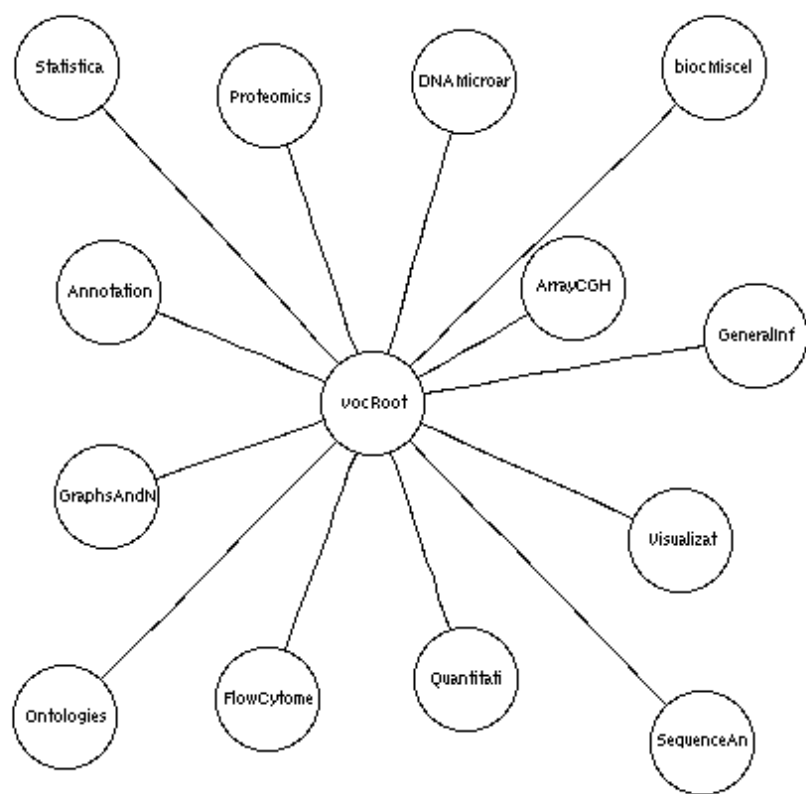


Figure 3: Top level terms.

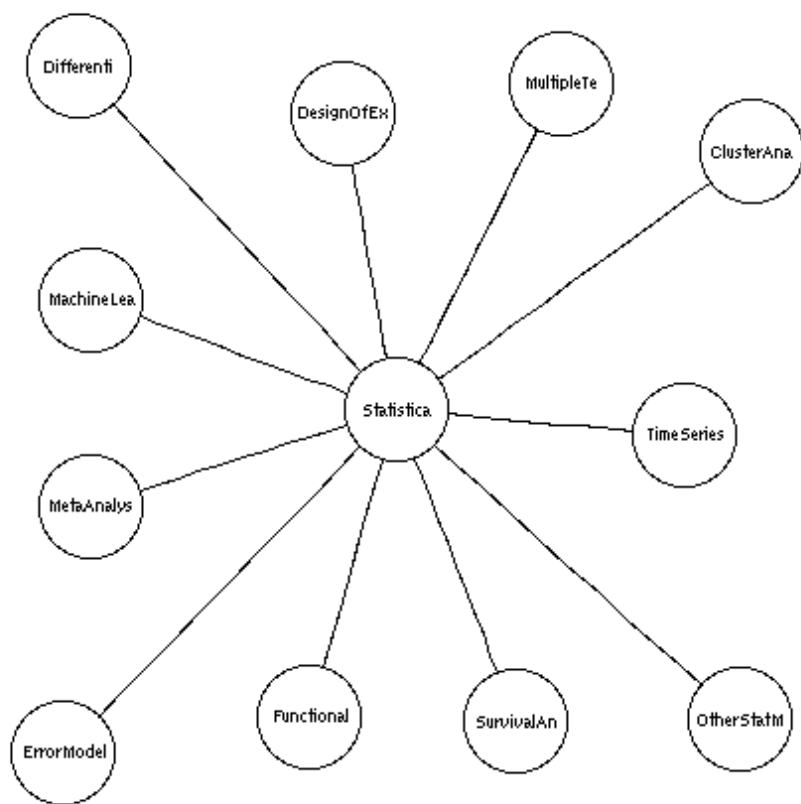


Figure 4: Terms subordinate to statistical modeling for high throughput biology.

6.3 An example ctv document

<CRANTaskView>

<name>MachineLearning</name>
<topic>Machine Learning & Statistical Learning</topic>
<maintainer>Torsten Hothorn</maintainer>

<info>

Several add-on packages implement ideas and methods developed at the borderline between computer science and statistics - this field of research is usually referred to as machine learning.

The packages can be roughly structured into the following topics:

<i>Neural Networks</i>: Single-hidden-layer neural network are implemented in package <tt>nnet</tt> as part of the <pkg>VR</pkg> bundle (shipped with base R).

<i>Recursive Partitioning</i>: Tree-structured models for regression, classification and survival analysis, following the ideas in the CART book, are implemented in <pkg>rpart</pkg> (shipped with base R) and <pkg>tree</pkg>. An adaptation of <pkg>rpart</pkg> for multivariate responses is available in package <pkg>mvp</pkg>. The validity of trees can be investigated via permutation approaches with package <pkg>rpart.permutation</pkg> and a tree algorithm fitting nearest neighbors in each node is implemented in package <pkg>knnTree</pkg>. For problems with binary input variables the package <pkg>LogicReg</pkg> implements logic regression. Graphical tools for the visualization of trees are available in packages <pkg>maptree</pkg> and <pkg>pinktoe</pkg>.

<i>Regularized and Shrinkage Methods</i>: Regression models with some constraint on the parameter estimates can be fitted with the <pkg>lasso2</pkg> and <pkg>lars</pkg> packages. The shrunken centroids classifier and utilities for gene expression analyses are implemented in package <pkg>pamr</pkg>.

<i>Random Forests</i>: The reference implementation of the random forest algorithm for regression and classification is available in package <pkg>randomForest</pkg>. Package <pkg>ipred</pkg> has bagging for regression, classification and survival analysis as well as bundling, a combination of multiple models via

- ensemble learning.
- Boosting**: Various forms of gradient boosting are implemented in packages `gbm` and `boost`.
- Support Vector Machines**: The function `svm()` from `e1071` offers an interface to the LIBSVM library and package `kernlab` implements a flexible framework for kernel learning (including SVMs, RVMs and other kernel learning algorithms). An interface to the SVMlight implementation (only for one-against-all classification) is provided in package `klaR`.
- Model selection and validation**: Package `e1071` has function `tune()` for hyper parameter tuning and function `errorest()` (`ipred`) can be used for error rate estimation. The cost parameter C for support vector machines can be chosen utilizing the functionality of package `svmpath`.

```
<packagelist>
  <pkg>boost</pkg>
  <pkg priority="core">e1071</pkg>
  <pkg priority="core">gbm</pkg>
  <pkg>ipred</pkg>
  <pkg priority="core">kernlab</pkg>
  <pkg>klaR</pkg>
  <pkg>lars</pkg>
  <pkg>lasso2</pkg>
  <pkg>mvpart</pkg>
  <pkg>pamr</pkg>
  <pkg>rpart.permutation</pkg>
  <pkg priority="core">randomForest</pkg>
  <pkg priority="core">rpart</pkg>
  <pkg>svmpath</pkg>
  <pkg>tree</pkg>
  <pkg priority="core">VR</pkg>
</packagelist>
```

```
<links>
  <a href="http://www.boosting.org/">Boosting Research Site</a>
</links>
```

</CRANTaskView>