Package ‘SomaticSignatures’

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Type Package
Title Somatic Signatures
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Description The SomaticSignatures package identifies mutational signatures of single nucleotide variants (SNVs). It provides a infrastructure related to the methodology described in Nik-Zainal (2012, Cell), with flexibility in the matrix decomposition algorithms.
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Suggests testthat, knitr, parallel,
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cluster-spectrum ......................................................... 2
derecomposition-signatures .............................................. 3
gcContent ........................................................................ 4
GRanges-converters ............................................................ 4
hs-chrs ........................................................................... 5
kmerFrequency .................................................................. 6
kmerFrequency ................................................................. 7
motif-functions ................................................................. 7
Cluster Mutational Spectrum

Description
Cluster the mutational spectrum by sample or motif.

Usage
clusterSpectrum(m, by = c("sample", "motif"), distance = "Cosine", ...)

Arguments
- m: Mutational spectrum matrix
- by: Dimension to cluster by.
- distance: Distance function used in the clustering.
- ...: Additional arguments passed to 'hclust'.

Details
Hierarchical clustering of the motif matrix aka mutational spectrum.

Value
An 'hclust' object.

See Also
- hclust
- dist
Description
Estimate somatic signatures from sequence motifs with a selection of statistical methods.

Usage
nmfDecomposition(x, r, ..., includeFit = FALSE)
pcaDecomposition(x, r, ..., includeFit = FALSE)

Arguments
x
GRanges object [required]
r
Number of signatures [integer, required]
... Additional arguments passed to 'NMF::nmf' or 'pcaMethods::pca'.
includeFit Include the fit object returned by the low-level decomposition function in the output.

Details
The 'nmfDecomposition' and 'pcaDecomposition' functions estimate a set of 'r' somatic signatures using the NMF or PCA, respectively.
In previous versions of the package, these functions were known as 'nmfSignatures' and 'pcaSignatures', respectively. While they are still available, we recommend using the new naming convention.

Value
The 'signature' functions return a list with the elements:
• wMatrix of the form 'motif x signature'
• hMatrix of the form 'sample x signature'
• vMatrix of the form 'motif x sample', containing the reconstruction of 'm' from 'w' and 'h'.
• mInput matrix 'm'
• rNumber of signatures.
• fitFit object returned by the low-level decomposition function, if 'includeFit' is true.

See Also
NMF package
pcaMethods package
prcomp
**gcContent**

**GC Content**

**Description**

Compute the GC content for regions of a reference sequence.

**Usage**

\[
gcContent(regions, ref)
\]

**Arguments**

- **regions**: GRanges object with the regions for which the GC content should be computed.
- **ref**: Reference sequence object, as a 'BSgenome' or 'FaFile' object.

**Value**

A numeric vector with the GC content [0,1] for each region.

**Examples**

```r
library(BSgenome.Hsapiens.1000genomes.hs37d5)
regs = GRanges(c("1", "2"), IRanges(1e7, width = 100))
gc = gcContent(regs, BSgenome.Hsapiens.1000genomes.hs37d5)
```

---

**GRanges-converters**

**GRanges converter functions**

**Description**

A set of utilities functions to convert and extract data in 'GRanges' objects.

**Usage**

- **ncbi(x)**
- **ucsc(x)**
- **seqchar(x)**

**Arguments**

- **x**: A 'GRanges' object or one inheriting from the 'GRanges' class [required].
Details

- grangesExtracts only the 'GRanges' information by dropping the metadata columns of the object. The 'seqinfo' slot is kept.
- ncbi, ucscShorthand for converting the seqnames notation to 'UCSC' (e.g. 'chr1', 'chrM') or 'NCBI' (e.g. '1', 'MT') notation, respectively. This also sets the 'genome' slot in the 'seqinfo' field to 'NA'.
- seqcharExtracts the 'seqnames' as a character vector.

Value

For 'ncbi', 'ucsc': An object of the same class as the input.
For 'seqchar': A character vector with 'seqnames'.

See Also

`seqnames`, `mcols`  
`seqlevelsStyle`

Examples

```r
mutect_path = system.file("examples", "mutect.tsv", package = "SomaticSignatures")
vr1 = readMutect(mutect_path, strip = TRUE)

## extract the GRanges
gr = granges(vr1)

## convert back and forth
gr_ncbi = ncbi(gr)
gr_ucsc = ucsc(gr_ncbi)
identical(gr, gr_ucsc)

## extract the seqnames as a character vector
seq_chars = seqchar(gr)
```

---

### hs-chrs

<table>
<thead>
<tr>
<th>Human Chromosome Names</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>

**Description**

List human chromosome names.

**Usage**

- `hsToplevel()`
- `hsAutosomes()`
- `hsAllosomes()`
- `hsLinear()`
kmerFrequency

Value

Character vector with chromosome names (NCBI notation).

Examples

hsToplevel()
hsAutosomes()
hsAllosomes()
hsLinear()

---

kmerFrequency                  Kmer Frequency

Description

Estimate the occurrence frequency of k-mers in a reference sequence.

Usage

kmerFrequency(ref, n = 1e4, k = 1, ranges = as(seqinfo(ref), "GRanges"))

Arguments

ref    A ‘BSgenome’ or ‘FaFile’ object matching the respective reference sequence [required].
n      The number of samples to draw [integer, default: 1e4].
k      The ‘k’-mer size of the context, including the variant position [integer, default: 3].
ranges Ranges in respect to the reference sequence to sample from [GRanges, default: take from the ‘seqinfo’ slot].

Details

The k-mer frequency is estimated by random sampling of `n` locations across the specified `ranges` of the reference sequence.

Value

A named vector, with names corresponding the the k-mer and value to the frequency.

Examples

library(BSgenome.Hsapiens.1000genomes.hs37d5)

kmer_freq = kmerFrequency(BSgenome.Hsapiens.1000genomes.hs37d5, 1e2, 3)
kmers-data

kmers-data  Kmer datasets

**Description**

3mer base frequencies of human whole-genome and whole-exome sampling, based on the hg19/GRCh37 reference sequence.

For details, see the ‘inst/scripts/kmers-data.R’ script.

**Value**

Vectors with frequency of k-mers.

**See Also**

kmerFrequency

**Examples**

```r
data(kmers, package = "SomaticSignatures")
```

---

motif-functions  Group somatic motifs

**Description**

Tabulate somatic motifs by a grouping variable.

**Usage**

```r
motifMatrix(vr, group = "sampleNames", normalize = TRUE)
```

**Arguments**

- `vr`: GRanges object [required]
- `group`: Grouping variable name [character, default: ‘sampleNames’]
- `normalize`: Normalize to frequency

**Details**

The `motifMatrix` function transforms the metadata columns of a `VRanges` object, as returned by the `mutationContext` function, to a matrix of the form ‘motifs x groups’. This constitutes the bases for the estimation of the signatures. By default (with ’normalize’ set to TRUE), the counts are transformed to frequencies, such that the sum of frequencies of each group equal 1. Otherwise (with ’normalize’ set to FALSE), the counts for each motif in a group is returned.
mutation-distribution

Value

Occurrence matrix with motifs in rows and samples in columns.

See Also

'mutationContext', 'mutationContextMutect'

Examples

```r
data(sca_motifs_tiny)

motifMatrix(sca_motifs_tiny, group = "study")
```

---

mutation-distribution  

Distributions of mutational locations.

Description

Summary and plotting function for characterizing the distributions of mutations along the genome.

Usage

```r
mutationDistance(x)

plotRainfall(x, group, size = 2, alpha = 0.5, space.skip = 0, ...)
```

Arguments

- `x`: A 'GRanges' or 'VRanges' object [required].
- `group`: The variable name for color groups [optional].
- `size`: Point size [default: 2]
- `alpha`: Alpha value for points [default: 0.5]
- `space.skip`: Space between chromosomes, as defined by 'plotGrandLinear' [default: 0]
- `...`: Additional arguments passed to 'plotGrandLinear'

Value

- `mutationDensity`: The position-sorted GRanges `x` with the additional column 'distance', specifying the distance from the previous mutation (or the beginning of the chromosome if it happens to be the first mutation on the chromosome.)
- `plotRainfall`: Object of class 'ggbio', as returned by 'plotGrandLinear'.

See Also

- `plotGrandLinear` from the 'ggbio' package
Examples

library(GenomicRanges)
library(IRanges)

set.seed(1)
chr_len = 100
gr = GRanges(rep(1:3, each = 10),
  IRanges(start = sample.int(chr_len, 30, replace = FALSE), width = 1),
  mutation = sample(c("A", "C", "G", "T"), 30, replace = TRUE))
seqlengths(gr) = rep(chr_len, 3)
p = plotRainfall(gr)
print(p)

mutational-normalization

Normalize Somatic Motifs

Description

Normalize somatic motifs, to correct for biases between samples.

Usage

normalizeMotifs(x, norms)

Arguments

x Matrix, as returned by 'motifMatrix' [required]
norms Vector with normalization factors [required]. The names must match the base sequence names in 'x'.

Value

A matrix as 'x' with normalized counts.

See Also

motifMatrix
**Mutational Plots**

**Description**

Plots for variant analysis

**Usage**

```r
plotVariantAbundance(x, group = NULL, alpha = 0.5, size = 2)
```

**Arguments**

- `x`: A VRanges object [required].
- `group`: Grouping variable, refers to a column name in `x`. By default, no grouping is performed.
- `alpha`: Alpha value for data points.
- `size`: Size value for data points.

**Details**

The `plotVariantAbundance` shows the variant frequency in relation to the total coverage at each variant position. This can be useful for examining the support of variant calls.

**Value**

A `ggplot` object.

---

**Estimate Somatic Signatures**

**Description**

Estimate somatic signatures from sequence motifs with a selection of statistical methods.

**Usage**

```r
identifySignatures(m, nSigs, decomposition = nmfDecomposition, ...)
```

**Arguments**

- `m`: Motif matrix, as returned by 'motifMatrix' [required].
- `nSigs`: Number of signatures [integer, required].
- `decomposition`: Function to apply for the matrix decomposition. The methods NMF and PCA are already implemented in the functions `nmfDecomposition` and `pcaDecomposition`, respectively.
- `...`: Additional arguments passed to the 'decomposition' function.
MutationalSignatures

Details

`identifySignatures` estimate a set of `r` somatic signatures, based on a matrix decomposition method (such as NMF, PCA).

Value

An object of class `MutationalSignatures`.

See Also

The predefined decomposition functions: `nmfDecomposition` and `pcaDecomposition`.

Examples

data("sca_mm", package = "SomaticSignatures")
sigs = identifySignatures(sca_mm, 5)

Description

Object representing of somatic signatures.

Usage

## S4 method for signature 'MutationalSignatures'
signatures(object)

## S4 method for signature 'MutationalSignatures'
samples(object)

## S4 method for signature 'MutationalSignatures'
observed(object)

## S4 method for signature 'MutationalSignatures'
fitted(object)

## S4 method for signature 'MutationalSignatures'
show(object)

Arguments

object `MutationalSignatures` object
Value

help("MutationalSignatures")

See Also

identifySignatures

mutationContext functions

Description

Extract the sequence context surrounding SNVs from a genomic reference.

Usage

mutationContext(vr, ref, k = 3, strand = FALSE, unify = TRUE, check = FALSE)
mutationContextMutect(vr, k = 3, unify = TRUE)

Arguments

vr

'VRanges' with SNV substitutions, with 'ref' and 'alt' columns filled [required]. Each element of 'ref' and 'alt' have be a single base from the DNA bases (A,C,G,T). For 'mutationContextMutect', an object as returned by the 'read-Mutect' function.

ref

A 'BSgenome', 'FaFile' or 'TwoBitfile' object representing the reference sequence [required]. More generally, any object with a defined 'getSeq' method can be used.

k

The 'k'-mer size of the context, including the variant position [integer, default: 3]. The variant will be located at the middle of the k-mer which requires 'k' to be odd.

strand

Should all variants be converted to the 'plus' strand? [logical, default: FALSE].

unify

Should the alterations be converted to have a C/T base pair as a reference alleles? [logical, default: TRUE]

check

Should the reference base of 'vr' be checked against 'ref' [logical, default: TRUE]? In case the two references do not match, a warning will be printed.

Details

The somatic motifs of a SNV, composed out of (a) the base change and (b) the sequence context surrounding the variant, is extracted from a genomic sequence with the 'mutationContext' function.

Different types of classes that represent the genomic sequence can used together with the 'mutationContext' function: 'BSgenome', 'FastaFile' and 'TwoBitFile' objects are supported through Bioconductor by default. See the vignette for examples discussing an analysis with non-reference genomes.

For mutect variant calls, all relevant information is already contained in the results and somatic motifs can constructed by using the 'mutationContextMutect' function, without the need for the reference sequence.
numberSignatures

Value
  The original 'VRanges' object 'vr', with the additional columns

alteration         DNAStringSet with 'ref|alt'.
context            DNAStringSet with '..N..' of length 'k', where N denotes the variant position.

See Also
  readMutect for mutationContextMutect
  'showMethods("getSeq")' for genomic references that can be used

Examples

mutect_path = system.file("examples", "mutect.tsv", package = "SomaticSignatures")
vr1 = readMutect(mutect_path)
ct1 = mutationContextMutect(vr1)

<table>
<thead>
<tr>
<th>numberSignatures</th>
<th>Number of Signatures</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description
  Assessment of the number of signatures in the data.

Usage
  assessNumberSignatures(m, nSigs, decomposition = nmfDecomposition, ..., nReplicates = 1)
  plotNumberSignatures(gof)

Arguments
  m             Mutational spectrum matrix, same as used for 'identifySignatures'.
  nSigs         Vector of integers with the numbers of signatures that should be tested. See the
                 'nSigs' argument for 'identifySignatures'.
  decomposition Function to apply for the matrix decomposition. See the 'decomposition' argument
                 for 'identifySignatures'.
  ...           Additional arguments passed to the 'decomposition' function. See the '...' argument
                 for 'identifySignatures'.
  nReplicates   How many runs should be used for assessing a value of 'nSigs'? For decomposition
                 methods with random seeding, values greater than 1 should be used.
  gof           Data frame, as returned of 'assessNumberSignatures'.


Details

Compute the decomposition for a given number of signatures, and assess the goodness of the reconstruction between the observed and fitted mutational spectra \( M \) and \( V \), respectively. The residual sum of squares (RSS)

\[
RSS = \sum_{i,j} (M_{ij} - V_{ij})^2
\]

and the explained variance

\[
ev = 1 - \frac{RSS}{\sum_{i,j} V_{ij}^2}
\]

are used as summary statistics which can generally applied to all decomposition approaches.

The 'plotNumberSignatures' function visualizes the results of the 'assessNumberSignatures' analysis. Statistics of the individual runs are shown as gray crosses, whereas the mean across the runs is depicted in red.

If a decomposition method uses random seeding and hence recomputing the decomposition of the same data can yield different results, evaluating the summary statistics will give more reliable estimates of the number of signatures. This applies to some NMF algorithms, for example. Methods with a deterministic decomposition, such as the standard PCA, do not need this, since repeated computations will yield the same decomposition. This behaviour is controlled by the 'nReplicates' parameter, where the default of '1' corresponds to a single run.

In practice, these summary statistics should not be trusted blindly, but rather interpreted together with biological knowledge and scientific reasoning. For a discussion of the interpretation of these statistics with special focus on the NMF decomposition, please refer to the references listed below.

Value
- assessNumberSignatures: A data frame with the RSS and explained variance for each run
- plotNumberSignatures: A ggplot object

References


See Also

identifySignatures
rss and evar functions of the NMF package.

Examples

data("sca_mm", package = "SomaticSignatures")
nSigs = 2:8
stat = assessNumberSignatures(sca_mm, nSigs, nReplicates = 3)
plotNumberSignatures(stat)
Description

Import `mutect` calls.

Usage

```r
readMutect(file, columns, strip = FALSE)
```

Arguments

- **file**: Location of the mutect tsv files [character, required]
- **columns**: Names of columns to import from the file [character vector, optional, default: missing]. If missing, all columns will be imported.
- **strip**: Should additional columns be imported? [logical, default: FALSE]. If TRUE, return only the bare `VRanges` object.

Details

The `readMutect` functions imports the mutational calls of a `*.tsv` file returned by the `mutect` caller to a `VRanges` object. For a description of the information of the columns, please refer to the mutect documentation.

Value

A `VRanges` object, with each row corresponding to one variant in the original file.

References


`http://www.broadinstitute.org/cancer/cga/mutect_run`

Examples

```r
mutect_path = system.file("examples", "mutect.tsv", package = "SomaticSignatures")
vr1 = readMutect(mutect_path)
vr2 = readMutect(mutect_path, strip = TRUE)
```
signature-plots

sca-data

SomaticCancerAlterations Results

Description
Motif matrix and 5 estimated signatures (NMF) from the somatic variant calls in the `SomaticCancerAlterations` package. For details, see the vignette of the `SomaticSignatures` package.

See Also
SomaticCancerAlterations package

Examples

```r
data(sca_motifs_tiny, package = "SomaticSignatures")
data(sca_mm, package = "SomaticSignatures")
data(sca_sigs, package = "SomaticSignatures")
```

signature-plots

Plot Mutational Signatures

Description
Visualize estimated signatures, sample contribution, and mutational spectra.

Usage

```r
plotObservedSpectrum(s, colorby = c("sample", "alteration"))
plotFittedSpectrum(s, colorby = c("sample", "alteration"))
plotMutationSpectrum(vr, group, colorby = c("sample", "alteration"), normalize = TRUE)
plotSignatureMap(s)
plotSignatures(s, normalize = FALSE, percent = FALSE)
plotSampleMap(s)
plotSamples(s, normalize = FALSE, percent = FALSE)
```

Arguments

- `s` MutationalSignatures object [required]
- `vr` VRanges object
- `colorby` Which variable to use for the coloring in the spectra representation.
- `normalize` Plot relative contributions (TRUE) instead of absolute (FALSE) ones.
- `percent` Display the results as fraction (FALSE) or percent (TRUE).
- `group` Charactering string that represents the variable name used for grouping.
Details

With the plotting function, the obtained signatures and their occurrence in the samples can be visualized either as a heatmap (’plotSignatureMap’, ’plotSampleMap’) or a barchart (’plotSignature’, ’plotSamples’).

Since the plotting is based on the ’ggplot2’ framework, all properties of the plots can be fully controlled by the user after generating the plots. Please see the examples for some customizations and the ’ggplot2’ documentation for the entire set of options.

Value

A ’ggplot’ object, whose properties can further be changed

See Also

See the ’ggplot2’ package for customizing the plots.

Examples

data(“sca_sigs”, package = “SomaticSignatures”)
plotSamples(sigs_nmf)
plotSignatures(sigs_nmf, normalize = TRUE)

# customize the plots ##
p = plotSamples(sigs_nmf)

library(ggplot2)
# (re)move the legend
p = p + theme(legend.position = ”none”)
# change the axis labels
p = p + xlab(“Studies”)
# add a title
p = p + ggtitle(“Somatic Signatures in TGCA WES Data”)
# change the color scale
p = p + scale_fill_brewer(palette = “Blues”)
# decrease the size of x-axis labels
p = p + theme(axis.text.x = element_text(size = 9))

p

Description

Published signatures, taken from ftp://ftp.sanger.ac.uk/pub/cancer/AlexandrovEtAl/signatures.txt

References

Examples

```r
data(signatures21, package = "SomaticSignatures")
head(signatures21)
```

---

### Description

Identifying somatic signatures of single nucleotide variants. This package provides a infrastructure related to the methodology described in Nik-Zainal (2012, Cell), with flexibility in the matrix decomposition algorithms.

### Details

The 'SomaticSignatures' package offers the framework for identifying mutational signatures of single nucleotide variants (SNVs) from high-throughput experiments. In the concept of mutational signatures, a base change resulting from an SNV is regarded in terms of motifs which embeds the variant in the context of the surrounding genomic sequence. Based on the frequency of such motifs across samples, mutational signatures and their occurrence in the samples can be estimated. An introduction into the methodology and a use case are illustrated in the vignette of this package.

### Author(s)


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### References


### Examples

```r
vignette(package = "SomaticSignatures")
```
**Description**

Utility functions

**Usage**

```r
dfConvertColumns(x, from = "character", to = "factor")
```

**Arguments**

- `x`: A 'data.frame' to convert [required].
- `from`: The class of the columns to be converted [default: 'character'].
- `to`: The class of the columns to be converted to [default: 'factor'].

**Details**

The `dfConvertColumns` converts all columns of a data frame with class `from` to the class `to`.

**Value**

A 'data.frame' object.
Index

*Topic IO
  readMutect, 15
*Topic datasets
  kmers-data, 7
  sca-data, 16
  signatures21-data, 17
*Topic manip
  GRanges-converters, 4
  mutationContext, 12
*Topic package
  SomaticSignatures, 18
*Topic utilities
  GRanges-converters, 4

assessNumberOfSignatures
  (numberSignatures), 13
cluster-spectrum, 2
decomposition-signatures, 3
dfConvertColumns (variants-utils), 19
dist, 2
evar, 14
findSignatures (mutational-signatures), 10
fitted (MutationalSignatures), 11
fitted, MutationalSignatures-method
  (MutationalSignatures), 11
gcContent, 4
GRanges-converters, 4
hclust, 2
hs-chrs, 5
hsAllosomes (hs-chrs), 5
hsAutosomes (hs-chrs), 5
hsLinear (hs-chrs), 5
hsToplevel (hs-chrs), 5
identifySignatures, 12, 14
identifySignatures
  (mutational-signatures), 10
k3we (kmers-data), 7
k3wg (kmers-data), 7
kmerFrequency, 6, 7
kmers (kmers-data), 7
kmers-data, 7
mcols, 5
motif-functions, 7
motifMatrix, 9, 11
motifMatrix (motif-functions), 7
mutation-distribution, 8
mutational-normalization, 9
mutational-plots, 10
mutational-signatures, 10
MutationalSignatures, 11, 11
MutationalSignatures-class
  (MutationalSignatures), 11
mutationContext, 11, 12
mutationContextMutect, 11
mutationContextMutect
  (mutationContext), 12
mutationDistance
  (mutation-distribution), 8
ncbi (GRanges-converters), 4
NMF, 3, 14
nmfDecomposition, 11
nmfDecomposition
  (decomposition-signatures), 3
nmfSignatures
  (decomposition-signatures), 3
normalizeMotifs
  (mutational-normalization), 9
numberSignatures, 13
observed (MutationalSignatures), 11
observed, MutationalSignatures-method
  (MutationalSignatures), 11
pcaDecomposition, 11
pcaDecomposition
  (decomposition-signatures), 3
pcaMethods, 3
pcaSignatures
  (decomposition-signatures), 3
plotFittedSpectrum (signature-plots), 16
plotGrandLinear, 8
plotMutationSpectrum (signature-plots), 16
plotNumberOfSignatures (numberSignatures), 13
plotObservedSpectrum (signature-plots), 16
plotRainfall (mutation-distribution), 8
plotSampleMap (signature-plots), 16
plotSamples (signature-plots), 16
plotSignatureMap (signature-plots), 16
plotSignatures (signature-plots), 16
plotVariantAbundance (mutational-plots), 10
prcomp, 3
readMutect, 13, 15
rss, 14
samples (MutationalSignatures), 11
samples, MutationalSignatures-method (MutationalSignatures), 11
sca-data, 16
sca_mm (sca-data), 16
sca_motifs_tiny (sca-data), 16
sca_sigs (sca-data), 16
seqchar (GRanges-converters), 4
seqlevelsStyle, 5
seqnames, 5
show (MutationalSignatures), 11
show, MutationalSignatures-method (MutationalSignatures), 11
signature-plots, 16
signatures (MutationalSignatures), 11
signatures, MutationalSignatures-method (MutationalSignatures), 11
signatures21 (signatures21-data), 17
signatures21-data, 17
sigs_nmf (sca-data), 16
sigs_pca (sca-data), 16
SomaticSignatures, 18
SomaticSignatures-package (SomaticSignatures), 18
ucsc (GRanges-converters), 4
variants-utils, 19