Package 'periodicDNA'

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Type Package

Title Set of tools to identify periodic occurrences of k-mers in DNA sequences

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Description This R package helps the user identify k-mers (e.g. di- or tri-nucleotides) present periodically in a set of genomic loci (typically regulatory elements). The functions of this package provide a straightforward approach to find periodic occurrences of k-mers in DNA sequences, such as regulatory elements. It is not aimed at identifying motifs separated by a conserved distance; for this type of analysis, please visit MEME website.

URL https://github.com/js2264/periodicDNA

BugReports https://github.com/js2264/periodicDNA/issues

RoxygenNote 7.1.0

Depends R (>= 4.0), Biostrings, GenomicRanges, IRanges, BSgenome, BiocParallel

Imports S4Vectors, rtracklayer, stats, GenomeInfoDb, magrittr, zoo, ggplot2, methods, parallel, cowplot

Suggests BSgenome.Scerevisiae.UCSC.sacCer3, BSgenome.Celegans.UCSC.ce11, BSgenome.Dmelanogaster.UCSC.dm6, BSgenome.Drerio.UCSC.danRer10, BSgenome.Hsapiens.UCSC.hg38, BSgenome.Mmusculus.UCSC.mm10, reticulate, testthat, covr, knitr, rmarkdown, pkgdown

VignetteBuilder knitr

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Contents

`ce11_all_REs` *ce11_all_REs*

Description

Regulatory elements annotated in C. elegans (ce11) according to Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv.

Usage

```
data(ce11_all_REs)
```

Format

GRanges

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_all_REs)
table(ce11_all_REs$regulatory_class)
table(ce11_all_REs$which.tissues)
```

`ce11_ATACseq` *ce11_ATACseq*

Description

Sample of ATAC-seq from mixed tissues in C. elegans young adults

Usage

```
data(ce11_ATACseq)
```

Format

RleList

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_ATACseq)
ce11_ATACseq
```

ce11_proms *ce11_proms*

Description

Promoters annotated in C. elegans (ce11) according to Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv.

Usage

```
data(ce11_proms)
```

Format

GRanges

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_proms)
table(ce11_proms$which.tissues)
```

ce11_proms_seqs *ce11_proms_seqs*

Description

Sample of sequences of promoters annotated in C. elegans (ce11) according to Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv.

Usage

```
data(ce11_proms_seqs)
```

Format

DNAStringSet

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_proms_seqs)
head(ce11_proms_seqs)
```

`ce11_TSSs` *ce11_TSSs*

Description

Coordinates of promoter TSSs annotated in C. elegans (ce11) used in Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv.

Usage

```
data(ce11_TSSs)
```

Format

GRanges

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_TSSs)
lengths(ce11_TSSs)
ce11_TSSs[[1]]
```

`ce11_WW_10bp` *ce11_WW_10bp*

Description

Sample of WW 10-bp periodicity track generated by getPeriodicityTrack() in ce11 over annotated accessible sites, with default parameters

Usage

```
data(ce11_WW_10bp)
```

Format

RleList

Source

BiorXiv

References

Serizay et al. 2020, "Tissue-specific profiling reveals distinctive regulatory architectures for ubiquitous, germline and somatic genes", BiorXiv. (DOI)

Examples

```
data(ce11_WW_10bp)
ce11_WW_10bp
```

`getPeriodicity` *A function to compute k-mer periodicity in sequence(s).*

Description

This function takes a set of sequences and a k-mer of interest, map a k-mer of interest in these sequences, computes all the pairwise distances (distogram), normalize it for distance decay, and computes the resulting power spectral density of the normalized distogram.

Usage

```
getPeriodicity(x, motif, ...)

## S3 method for class 'DNAStringSet'
getPeriodicity(
  x,
  motif,
  range_spectrum = seq(1, 200),
  BPPARAM = setUpBPPARAM(1),
  roll = 3,
  verbose = TRUE,
  sample = 0,
  n_shuffling = 0,
  cores_shuffling = 1,
  cores_computing = 1,
  order = 1,
  ...
)

## S3 method for class 'GRanges'
getPeriodicity(x, motif, genome = "BSgenome.Celegans.UCSC.ce11", ...)

## S3 method for class 'DNAString'
getPeriodicity(x, motif, ...)
```

Arguments

x	a DNAString, DNAStringSet or GRanges object.
motif	a k-mer of interest
...	Arguments passed to S3 methods
range_spectrum	Numeric vector Range of the distogram to use to run the Fast Fourier Transform on (default: 1:200, i.e. all pairs of k-mers at a maximum of 200 bp from each other).
BPPARAM	split the workload over several processors using BiocParallel
roll	Integer Window to smooth the distribution of pairwise distances (default: 3, to discard the 3-bp periodicity of dinucleotides which can be very strong in vertebrate genomes)
verbose	Boolean
sample	Integer if > 0, will randomly sample this many integers from the dists vector before normalization. This ensures consistency when looking at periodicity in different genomes, since different genomes will have different GC percent
n_shuffling	Integer, how many times should the sequences be shuffled? (default = 0)
cores_shuffling	integer, Number of cores used for shuffling (used if n_shuffling > 0)

`cores_computing` integer, split the workload over several processors using BiocParallel (used if n_shuffling > 0)

`order` Integer, which order to take into consideration for shuffling (ushuffle python library must be installed for orders > 1) (used if n_shuffling > 0)

`genome` genome ID, BSgenome or DNAStringSet object (optional, if x is a GRanges)

Value

A list containing the results of getPeriodicity function.

- The dists vector is the raw vector of all distances between any possible k-mer.
- The hist data.frame is the distribution of distances over range_spectrum.
- The normalized_hist is the raw hist, normalized for decay over increasing distances.
- The spectra object is the output of the FFT applied over normalized_hist.
- The PSD data frame is the power spectral density scores over given frequencies.
- The motif object is the k-mer being analysed.
- The final periodicity metrics computed by getPeriodicity()

If getPeriodicity() is ran with n_shuffling > 0, the resulting list also contains PSD values computed when iterating through shuffled sequences.

Methods (by class)

- `DNAStringSet`: S3 method for DNAStringSet
- `GRanges`: S3 method for GRanges
- `DNAString`: S3 method for DNAString

Examples

```
data(ce11_proms_seqs)
periodicity_result <- getPeriodicity(
    ce11_proms_seqs[1:100],
    motif = 'TT'
)
head(periodicity_result$PSD)
plotPeriodicityResults(periodicity_result)
#
data(ce11_TSSs)
periodicity_result <- getPeriodicity(
    ce11_TSSs[['Ubiq.']][1:10],
    motif = 'TT',
    genome = 'BSgenome.Celegans.UCSC.ce11'
)
head(periodicity_result$PSD)
plotPeriodicityResults(periodicity_result)
#
data(ce11_TSSs)
periodicity_result <- getPeriodicity(
```

```
    ce11_TSSs[['Ubiq.']][1:10],
    motif = 'TT',
    genome = 'BSgenome.Celegans.UCSC.ce11',
    n_shuffling = 10
)
head(periodicity_result$PSD)
plotPeriodicityResults(periodicity_result)
```

`getPeriodicityTrack` *Function to generate a k-mer periodicity track*

Description

This function takes a set of GRanges in a genome, recover the corresponding sequences and divides them using a sliding window. For each sub-sequence, it then computes the PSD value of a k-mer of interest at a chosen period, and generates a linear .bigWig track from these values.

Usage

```
getPeriodicityTrack(
  genome = NULL,
  granges,
  motif = "WW",
  period = 10,
  BPPARAM = setUpBPPARAM(1),
  extension = 1000,
  window_size = 100,
  step_size = 2,
  range_spectrum = seq(5, 50),
  smooth_track = 20,
  bw_file = NULL
)
```

Arguments

`genome`	DNAStringSet, BSgenome or genome ID
`granges`	GRanges object
`motif`	character, k-mer of interest.
`period`	Integer, the period of the k-mer to study (default=10).
`BPPARAM`	split the workload over several processors using BiocParallel
`extension`	Integer, the width the GRanges are going to be extended to (default 1000).
`window_size`	Integer, the width of the bins to split the GRanges objects in (default 100).
`step_size`	Integer, the increment between bins over GRanges (default 2).
`range_spectrum`	Numeric vector, the distances between nucleotides to take into consideration when performing Fast Fourier Transform (default seq_len(50)).
`smooth_track`	Integer, smooth the resulting track
`bw_file`	character, the name of the output bigWig track

Value

Rlelist and a bigWig track in the working directory.

Examples

```
data(ce11_proms)
track <- getPeriodicityTrack(
    genome = 'BSgenome.Celegans.UCSC.ce11',
    ce11_proms[1],
    extension = 200,
    window_size = 100,
    step_size = 10,
    smooth_track = 1,
    motif = 'WW',
    period = 10,
    BPPARAM = setUpBPPARAM(1)
)
track
unlink(
    'BSgenome.Celegans.UCSC.ce11_WW_10-bp-periodicity_g-100^10_smooth-1.bw'
)
```

---

getPeriodicityWithIterations

A function to compute PSDs with iterations

Description

This function computes PSD values of a given k-mer of interest in a set of input sequences. It also iterates the PSD calculation process over shuffled sequences, if n_shuffling is used.

Usage

```
getPeriodicityWithIterations(x, ...)

## S3 method for class 'DNAStringSet'
getPeriodicityWithIterations(
  x,
  motif,
  n_shuffling = 10,
  cores_shuffling = 1,
  cores_computing = 1,
  order = 1,
  verbose = 1,
  ...
)

## S3 method for class 'GRanges'
getPeriodicityWithIterations(x, genome, ...)
```

Arguments

x	DNAStringSet, sequences of interest
...	Arguments passed to S3 methods
motif	character, k-mer of interest
n_shuffling	integer, Number of shuffling
cores_shuffling	integer, Number of cores used for shuffling
cores_computing	integer, split the workload over several processors using BiocParallel
order	Integer, which order to take into consideration for shuffling (ushuffle python library must be installed for orders > 1)
verbose	integer, Should the function be verbose?
genome	genome ID, BSgenome or DNAStringSet object (optional, if x is a GRanges)

Value

Several metrics

Methods (by class)

- `DNAStringSet`: S3 method for DNAString
- `GRanges`: S3 method for GRanges

Examples

```
data(ce11_proms_seqs)
res <- getPeriodicityWithIterations(
    ce11_proms_seqs[1:10],
    genome = 'BSgenome.Celegans.UCSC.ce11',
    motif = 'TT',
    cores_shuffling = 1
)
res$observed_PSD
res$shuffled_PSD
```

`plotAggregateCoverage` *A function to plot aggregated signals over sets of GRanges*

Description

This function takes one or several RleList genomic tracks (e.g. imported by rtraklayer::import(..., as = 'Rle')) and one or several GRanges objects. It computes coverage of the GRanges by the genomic tracks and returns an aggregate coverage plot.

Usage

```
plotAggregateCoverage(x, ...)

## S3 method for class 'CompressedRleList'
plotAggregateCoverage(x, granges, ...)

## S3 method for class 'SimpleRleList'
plotAggregateCoverage(
  x,
  granges,
  colors = NULL,
  xlab = "Center of elements",
  ylab = "Score",
  xlim = NULL,
  ylim = NULL,
  quartiles = c(0.025, 0.975),
  verbose = FALSE,
  bin = 1,
  plot_central = TRUE,
  run_in_parallel = FALSE,
  split_by_granges = FALSE,
  norm = "none",
  ...
)

## S3 method for class 'list'
plotAggregateCoverage(
  x,
  granges,
  colors = NULL,
  xlab = "Center of elements",
  ylab = "Score",
  xlim = NULL,
  ylim = NULL,
  quartiles = c(0.025, 0.975),
  verbose = FALSE,
  bin = 1,
  plot_central = TRUE,
  split_by_granges = TRUE,
  split_by_track = FALSE,
  free_scales = FALSE,
  run_in_parallel = FALSE,
  norm = "none",
  ...
)
```

Arguments

x	a single signal track (CompressedRleList or SimpleRleList class), or several signal tracks (SimpleRleList or CompressedRleList class) grouped in a named list
...	additional parameters
granges	a GRanges object or a named list of GRanges
colors	a vector of colors
xlab	x axis label
ylab	y axis label
xlim	y axis limits
ylim	y axis limits
quartiles	Which quantiles to use to determine y scale automatically?
verbose	Boolean
bin	Integer Width of the window to use to smooth values by zoo::rollMean
plot_central	Boolean Draw a vertical line at 0
run_in_parallel	Boolean Should the plots be computed in parallel using mclapply?
split_by_granges	Boolean Facet plots over the sets of GRanges
norm	character Should the signal be normalized ('none', 'zscore' or 'log2')?
split_by_track	Boolean Facet plots by the sets of signal tracks
free_scales	Boolean Should each facet have independent y-axis scales?

Value

An aggregate coverage plot.

Methods (by class)

- `CompressedRleList`: S3 method for CompressedRleList
- `SimpleRleList`: S3 method for SimpleRleList
- `list`: S3 method for list

Examples

```
data(ce11_ATACseq)
data(ce11_WW_10bp)
data(ce11_proms)

p1 <- plotAggregateCoverage(
    ce11_ATACseq,
    resize(ce11_proms[1:100], fix = 'center', width = 1000)
)
p1
```

```
proms <- resize(ce11_proms[1:100], fix = 'center', width = 400)
p2 <- plotAggregateCoverage(
    ce11_ATACseq,
    list(
        'Ubiq & Germline promoters' =
            proms[proms$which.tissues %in% c('Ubiq.', 'Germline')],
        'Other promoters' =
            proms[!(proms$which.tissues %in% c('Ubiq.', 'Germline'))]
    )
)
p2

p3 <- plotAggregateCoverage(
    list(
        'atac' = ce11_ATACseq,
        'WW_10bp' = ce11_WW_10bp
    ),
    proms,
    norm = 'zscore'
)
p3

p4 <- plotAggregateCoverage(
    list(
        'ATAC-seq' = ce11_ATACseq,
        'WW 10-bp periodicity' = ce11_WW_10bp
    ),
    list(
        'Ubiq & Germline promoters' =
            proms[proms$which.tissues %in% c('Ubiq.', 'Germline')],
        'Other promoters' =
            proms[!(proms$which.tissues %in% c('Ubiq.', 'Germline'))]
    ),
    norm = 'zscore'
)
p4

p5 <- plotAggregateCoverage(
    list(
        'ATAC-seq' = ce11_ATACseq,
        'WW 10-bp periodicity' = ce11_WW_10bp
    ),
    list(
        'Ubiq & Germline promoters' =
            proms[proms$which.tissues %in% c('Ubiq.', 'Germline')],
        'Other promoters' =
            proms[!(proms$which.tissues %in% c('Ubiq.', 'Germline'))]
    ),
    split_by_granges = FALSE,
    split_by_track = TRUE,
    norm = 'zscore'
)
```

```
p5
```

`plotPeriodicityResults` *Plot the output of getPeriodicity()*

Description

This function plots some results from the result of getPeriodicity(). It plots the raw distogram, the distance-decay normalized distogram and the resulting PSD values. If a shuffled control has been performed by getPeriodicity(), it also displays it.

Usage

```
plotPeriodicityResults(
  results,
  periods = c(2, 20),
  filter_periods = TRUE,
  facet_control = TRUE,
  xlim = NULL,
  fdr_threshold = 0.05,
  ...
)
```

Arguments

`results`	The output of getPeriodicity function.
`periods`	Vector a numerical vector of length 2, to specify the x-axis limits
`filter_periods`	Boolean Should the x-axis be constrained to the periods?
`facet_control`	Boolean should the shuffling plots be faceted?
`xlim`	Integer x axis upper limit in raw and norm. distograms
`fdr_threshold`	Float, significance threshold
`...`	Additional theme arguments passed to theme_ggplot2()

Value

list A list containing four ggplots

Examples

```
data(ce11_TSSs)
periodicity_result <- getPeriodicity(
    ce11_TSSs[['Ubiq.']][1:100],
    genome = 'BSgenome.Celegans.UCSC.ce11',
    motif = 'TT',
    BPPARAM = setUpBPPARAM(1)
```

```
)
head(periodicity_result$PSD)
plotPeriodicityResults(periodicity_result)
plotPeriodicityResults(periodicity_result, xlim = 150)
plotPeriodicityResults(
    periodicity_result, xlim = 150, filter_periods = FALSE
)
plotPeriodicityResults(
    periodicity_result, xlim = 150, facet_control = FALSE
)
```

`setUpBPPARAM` *setUpBPPARAM*

Description

A function to dynamically select MulticoreParam or SnowParam (if Windows)

Usage

```
setUpBPPARAM(nproc = 1)
```

Arguments

`nproc`	number of processors

Value

A BPPARAM object

Examples

```
BPPARAM <- setUpBPPARAM(1)
```

`theme_ggplot2` *Personal ggplot2 theming function, adapted from roboto-condensed at https://github.com/hrbrmstr/hrbrthemes/*

Description

Personal ggplot2 theming function, adapted from roboto-condensed at https://github.com/hrbrmstr/hrbrthemes/

Usage

```
theme_ggplot2(
  grid = TRUE,
  border = TRUE,
  base_size = 8,
  plot_title_size = 12,
  plot_title_face = "plain",
  plot_title_margin = 5,
  subtitle_size = 11,
  subtitle_face = "plain",
  subtitle_margin = 5,
  strip_text_size = 10,
  strip_text_face = "bold",
  caption_size = 9,
  caption_face = "plain",
  caption_margin = 3,
  axis_text_size = base_size,
  axis_title_size = 9,
  axis_title_face = "plain",
  axis_title_just = "rt",
  panel_spacing = grid::unit(2, "lines"),
  grid_col = "#cccccc",
  plot_margin = margin(12, 12, 12, 12),
  axis_col = "#cccccc",
  axis = FALSE,
  ticks = FALSE
)
```

Arguments

`grid`	panel grid ('TRUE', 'FALSE', or a combination of 'X', 'x', 'Y', 'y')
`border`	border if 'TRUE' add border
`base_size`	base font size
`plot_title_size`, `plot_title_margin`	plot title size and margin
`plot_title_face`	plot title face
`subtitle_face`, `subtitle_size`	plot subtitle face and size
`subtitle_margin`	plot subtitle margin bottom (single numeric value)
`strip_text_face`, `strip_text_size`	facet label font face and size
`caption_face`, `caption_size`, `caption_margin`	plot caption face, size and margin
`axis_text_size`	font size of axis text

`axis_title_face`, `axis_title_size`
: axis title font face and size

`axis_title_just`
: axis title font justificationk one of '[blmcrt]'

`panel_spacing`
: panel spacing (use 'unit()')

`grid_col`
: grid color

`plot_margin`
: plot margin (specify with [ggplot2::margin])

`axis_col`
: axis color

`axis`
: add x or y axes? 'TRUE', 'FALSE', "'xy'"

`ticks`
: ticks if 'TRUE' add ticks

Value

theme A ggplot theme

Examples

```
library(ggplot2)

ggplot(mtcars, aes(mpg, wt)) +
  geom_point() +
  labs(x="Fuel effiency (mpg)", y="Weight (tons)",
       title="Seminal ggplot2 scatterplot example") +
  theme_ggplot2()
```

Index