Package ‘periodicDNA’

April 9, 2024

Type Package

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

Version 1.12.0

Date 2021-11-21

Encoding UTF-8

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

biocViews SequenceMatching, MotifDiscovery, MotifAnnotation, Sequencing, Coverage, Alignment, DataImport

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git_url https://git.bioconductor.org/packages/periodicDNA

Usage

data(ce11_all_REs)

Format

GRanges

Source

BiorXiv
References

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

Examples

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

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 ubiquituous, germline and somatic genes", BiorXiv. (DOI)

Examples

data(ce11_ATACseq)
ce11_ATACseq
Description


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)

Description


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)

data(ce11_TSSs)
lengths(ce11_TSSs)

Description


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]]
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)
getPeriodicity

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)

geno_ome
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(cell_proms_seq)
periodicity_result <- getPeriodicity(
  cell_proms_seq[1:100],
  motif = 'TT'
)
head(periodicity_result$PSD)
plotPeriodicYResults(periodicity_result)
#
data(cell_TSSs)
periodicity_result <- getPeriodicity(
  cell_TSSs[['Ubiq.']][1:10],
  motif = 'TT',
  genome = 'BSgenome.Celegans.UCSC.cell'
)
head(periodicity_result$PSD)
plotPeriodicYResults(periodicity_result)
#
data(cell_TSSs)
periodicity_result <- getPeriodicity(}
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

gene

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
getPeriodicityWithIterations

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, ...)
**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.

**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**

```r
data(cell_proms_seq)
res <- getPeriodicityWithIterations(
  cell_proms_seq[1:10],
  genome = 'BSgenome.Celegans.UCSC.cell',
  motif = 'TT',
  cores_shuffling = 1
)
res$observed_PSD
res$shuffled_PSD
```
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",
  ...
)
plotAggregateCoverage

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(cell_ATACseq)
data(cell_WW_10bp)
data(cell_proms)

pl <- plotAggregateCoverage(
  cell_ATACseq,
  resize(cell_proms[1:100], fix = 'center', width = 1000)
)

pl
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'
)
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

**Description**

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

**Usage**

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

**Arguments**

- `nproc`: number of processors

**Value**

A BPPARAM object

**Examples**

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

---

### theme_ggplot2

**Description**

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

---

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

**Usage**

```r
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 size and margin
- **plot_title_face**: plot title face
- **plot_title_margin**: plot title margin
- **subtitle_size**: plot subtitle size
- **subtitle_face**: plot subtitle face
- **subtitle_margin**: plot subtitle margin bottom (single numeric value)
- **strip_text_size**: facet label font face and size
- **strip_text_face**: facet label font face
- **caption_size**: plot caption size
- **caption_face**: plot caption face
- **caption_margin**: plot caption margin
- **axis_text_size**: font size of axis text
- **axis_title_size**: font size of axis title
- **axis_just**: justification of axis title
- **panel_spacing**: spacing between panels
- **grid_col**: color of grid
- **plot_margin**: margin around plot
- **axis_col**: color of axis
- **axis**: show axis
- **ticks**: show ticks
theme_ggplot2

axis_title_face, axis_title_size
axis title font face and size

axis_title_just
axis title font justificationk one of ‘[blmcr]’

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 efficiency (mpg)", y="Weight (tons)",
       title="Seminal ggplot2 scatterplot example") +
  theme_ggplot2()
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