Package ‘seqArchR’

May 3, 2024

Type Package
Title Identify Different Architectures of Sequence Elements
Version 1.8.0
Description seqArchR enables unsupervised discovery of _de novo_ clusters with characteristic sequence architectures characterized by position-specific motifs or composition of stretches of nucleotides, e.g., CG-richness. seqArchR does _not_ require any specifications w.r.t. the number of clusters, the length of any individual motifs, or the distance between motifs if and when they occur in pairs/groups; it directly detects them from the data. seqArchR uses non-negative matrix factorization (NMF) as its backbone, and employs a chunking-based iterative procedure that enables processing of large sequence collections efficiently. Wrapper functions are provided for visualizing cluster architectures as sequence logos.

License GPL-3 | file LICENSE

URL https://snikumbh.github.io/seqArchR/,
https://github.com/snikumbh/seqArchR

BugReports https://github.com/snikumbh/seqArchR/issues

SystemRequirements Python (>= 3.5), scikit-learn (>= 0.21.2), packaging

Depends R (>= 4.2.0)
Imports utils, graphics, cvTools (>= 0.3.2), MASS, Matrix, methods, stats, cluster, matrixStats, fpc, cli, prettyunits, reshape2 (>= 1.4.3), reticulate (>= 1.22), BiocParallel, Biostrings, grDevices, ggplot2 (>= 3.1.1), ggseqlogo (>= 0.1)

Suggests cowplot, hopach (>= 2.42.0), BiocStyle, knitr (>= 1.22), rmarkdown (>= 1.12), testthat (>= 3.0.2), covr, vdiff (>= 0.3.0)

VignetteBuilder knitr

biocViews MotifDiscovery, GeneRegulation, MathematicalBiology, SystemsBiology, Transcriptomics, Genetics, Clustering, DimensionReduction, FeatureExtraction, DNASeq
**collate_clusters**

**Description**

Collate sequences original divided across n clusters into a new set of m clusters. These ‘m’ clusters obtained by clustering the original ‘n’ clusters. Assume a collection of 100 sequences across seven existing clusters. These seven clusters are collated to obtain three resulting clusters. Collating 100 sequences distributed across the seven clusters into the resulting three clusters can be achieved with `collate_clusters`. 

---

**Encoding** UTF-8  
**LazyData** false  
**RoxygenNote** 7.2.1  
**git_url** https://git.bioconductor.org/packages/seqArchR  
**git_branch** RELEASE_3_19  
**git_last_commit** 3c13d82  
**git_last_commit_date** 2024-04-30  
**Repository** Bioconductor 3.19  
**Author** Sarvesh Nikumbh [aut, cre, cph]  
**Maintainer** Sarvesh Nikumbh <sarvesh.nikumbh@gmail.com>  
**Contents**

- collate_clusters ........................................... 2  
- collate_seqArchR_result .................................. 3  
- get_clBasVec .............................................. 5  
- get_one_hot_encoded_seqs .................................. 6  
- get_seqs_clust_list ........................................ 7  
- make_PWMs .................................................. 8  
- plot_arch_for_clusters .................................... 9  
- plot_ggseqlogo_of_seqs ................................... 10  
- prepare_data_from_FASTA ................................. 12  
- seqArchR ................................................... 13  
- seqs_str .................................................... 16  
- set_config ................................................ 17  
- viz_bas_vec ............................................... 19  
- viz_pwm .................................................... 20  
- viz_seqs_acgt_mat ....................................... 22  

---

**Index**

- collate_clusters .......................... 24  

**collate_clusters**

Collate sequence IDs from an existing clustering according to a new, given clustering of the existing clusters.
Usage

collate_clusters(to_clust, orig_clust)

Arguments

to_clust A list giving clustering of factors. In other words this is the clustering of clusters of sequences given in `orig_clust`

orig_clust A list of sequence IDs in existing clusters

Value

A list with sequence IDs collated by the specified clustering

Examples

set.seed(123)
n <- 7; nn <- 100
orig_clust_labels <- ceiling(n * runif(nn))
orig_clust <- seqArchR::get_seqs_clust_list(orig_clust_labels)
to_clust <- list(c(1,4), c(2,3,5), c(6,7))
collate_clusters(to_clust = to_clust, orig_clust = orig_clust)

Description

We use hierarchical clustering for reordering/collating raw clusters from seqArchR’s given iteration.

Usage

collate_seqArchR_result(  
result,  
iter = length(result$seqsClustLabels),  
clust_method = "hc",  
aggl_method = "ward.D",  
dist_method = "euclid",  
regularize = FALSE,  
topn = 50,  
collate = TRUE,  
return_order = FALSE,  
flags = list(debugFlag = FALSE, verboseFlag = TRUE),  
)
collate_seqArchR_result

Arguments

result
The seqArchR result object.

iter
Specify clusters at which iteration of seqArchR are to be reordered/collated. Default is the last iteration of the seqArchR result object.

clust_method
Specify 'hc' for hierarchical clustering. Currently, only hierarchical clustering is supported.

aggl_method
One of linkage values as specified for hierarchical clustering with hclust. Default is 'ward.D'.

dist_method
Distance measure to be used with hierarchical clustering. Available options are "euclid" (default), "cor" for correlation, "cosangle" for cosine angle.

regularize
Logical. Specify TRUE if regularization is to be performed before comparison. Default is FALSE. Also see argument 'topN'.

topn
Use only the top N dimensions of each basis vector for comparing them. Note that since each basis vector has 4L or 16L (mono- or dinucleotides) dimensions, each dimension is a combination of nucleotide and its position in the sequence. This argument selects the top N dimensions of the basis vector. This is ignored when argument 'regularize' is FALSE.

collate
Logical. Specify TRUE if collation using hierarchical agglomerative clustering is to be performed, otherwise FALSE.

return_order
Logical. Use this argument when you want hierarchical clustering to be performed but not collation of clusters. Therefore, setting return_order to TRUE will return the hierarchical clustering object itself. This enables custom downstream processing/analysis.

flags
Pass the flags object similar to the flags in configuration of the seqArchR result object.

Value

When 'collate' is TRUE, a list with the following elements is returned:

- **basisVectorsCLust** A list storing collation information of the basis vectors, i.e, IDs of basis vectors that were collated into one.
- **clusters** A list of sequences in each collated cluster.
- **seqClustLabels** Cluster labels for all sequences according to the collated clustering.

When 'collate' is FALSE, it returns the already existing basis vectors, each as singleton clusters. The sequence cluster labels and sequence clusters are also handled accordingly. All are available as part of the same list as the earlier case.

When 'return_order' is set to TRUE, the hierarchical clustering result is returned instead.
get_clBasVec

Examples

```r
res <- readRDS(system.file("extdata", "example_seqArchRresult.rds", 
    package = "seqArchR", mustWork = TRUE))

# While the default settings for collation use Euclidean distance and
# ward.D agglomeration, one can choose to use different settings, say,
# correlation distance and complete linkage, and also regularizing to use
# only top 50 dimensions (nucleotide-positions combinations)
collated_res <- collate_seqArchR_result(result = res, iter = 2, 
    aggl_method = "complete", dist_method = "cor", 
    regularize = TRUE, topn = 50)

names(collated_res)
```

---

### Description

Basis vectors’ information for the selected iteration.

### Usage

```r
get_clBasVec(res, iter)
get_clBasVec_k(res, iter)
get_clBasVec_m(res, iter)
get_seqClLab(res, iter = NULL)
```

### Arguments

- **res**: seqArchR result object.
- **iter**: Choose the iteration of seqArchR result to get from.

### Value

- **get_clBasVec**: A list with two elements ‘nBasisVectors’ (integer) and ‘basisVectors’ (matrix).
- **get_clBasVec_k**: The number of basis vectors (integer).
- **get_clBasVec_m**: The basis vectors’ matrix with features along the rows of the matrix.
- **get_seqClLab**: A character vector denoting the cluster IDs for each sequence.
get_one_hot_encoded_seqs

Description
Get one-hot encoded sequences

Usage
get_one_hot_encoded_seqs(seqs, sinuc_or_dinuc = "sinuc")

Arguments
seqs A DNAStringSet object holding the given DNA sequences
sinuc_or_dinuc character string, 'sinuc' or 'dinuc' to select for mono- or dinucleotide profiles.

Value
A sparse matrix of sequences represented with one-hot-encoding
get_seqs_clust_list

Retrieve sequence clusters as a list from the sequence labels

Description
Given the sequence cluster labels from the seqArchR result object, returns the clusters separated as a list.

Usage
get_seqs_clust_list(seqs_clust_lab)

Arguments
seqs_clust_lab  Sequences with cluster labels as in the seqArchR result object.

Value
A list holding sequence IDs belonging in each cluster.

Examples
clustLabels <- sample(seq_len(4), 50, replace = TRUE)
print(clustLabels)
geq_seqs_clust_list(clustLabels)
make_PWMs

Make a PWM-resembling matrix out of a given n-vector

Description

The given matrix (or simply a vector) is reshaped to have four rows for four nucleotides and a relevant number of columns.

Usage

make_PWMs(vec, add_pseudo_counts = TRUE, scale = TRUE, sinuc = TRUE)

Arguments

vec

A vector that will be reshaped into a PWM matrix of DNA sequences. Note that the matrix is formed by row.

add_pseudo_counts

Logical, taking values TRUE or FALSE, specifying whether or not pseudo-counts are added to the matrix.

scale

Logical, taking values TRUE or FALSE, specifying whether or not the matrix is scaled column-wise, i.e., all columns summed to 1.

sinuc

Logical. Specify TRUE for mononucleotides (default), FALSE to for dinucleotides.

Value

A PWM. If sinuc is ‘TRUE’, the PWM has 4 rows corresponding to the 4 nucleotides (A, C, G, T) and the relevant number of columns (i.e., number of elements in given vector/4). If dinucleotide is selected, by setting ‘sinuc’ to ‘FALSE’, the PWM has 16 rows corresponding to the dinucleotide combinations of the four nucleotides (A, C, G, T) and the relevant number of columns (i.e., number of elements in given vector/16).

Examples

## Mononucleotides case
## Make a dummy PWM of dimensions 4 * 10 from a vector
vec <- runif(4*10)
pwm <- seqArchR::make_PWMs(vec = vec, add_pseudo_counts = FALSE)

## Dinucleotides case
res <- readRDS(system.file("extdata", "example_seqArchRresult.rds",
    package = "seqArchR", mustWork = TRUE))
pwm <- seqArchR::make_PWMs(get_clBasVec_m(res, iter=1)[,1],
    add_pseudo_counts = FALSE, sinuc = FALSE)
**Description**

Given a collection of FASTA sequences as a DNAStringSet object, and the clusters information, this function plots the architectures for all clusters. If a name for the PDF file is provided, the resulting set of architecture sequence logos are saved as a multi-page PDF.

**Usage**

```r
plot_arch_for_clusters(
  seqs,
  clust_list,
  pos_lab = NULL,
  xt_freq = 5,
  set_titles = TRUE,
  pdf_width = 11,
  pdf_height = 2,
  pdf_name = NULL,
  show = FALSE,
  ...
)
```

**Arguments**

- **seqs**: Sequences as a DNAStringSet.
- **clust_list**: Clusters as a list of sequence IDs in each cluster.
- **pos_lab**: Labels for sequence positions, should be of same length as that of the sequences. Default value is NULL, when the positions are labeled from 1 to the length of the sequences.
- **xt_freq**: Frequency of x-axis ticks.
- **set_titles**: Specify TRUE if titles are to be written for the plots. With FALSE, there are no titles for the plots. The title for each plot includes the current cluster number, total number of clusters, start and end sequence numbers in the collection.
- **pdf_width, pdf_height**: Width and height in inches of the PDF file. Default values are 11 and 2.
- **pdf_name**: Specify the PDF filename.
- **show**: Set TRUE if plot should be immediately shown/plotted. Default is TRUE. By setting FALSE, one can simply collect the list of plots and use any other approach to arrange/display them. See examples.
- **...**: Additional args passed to `plot_ggseqlogo_of_seqs`. 

---

---
Value

A list of (ggplot2-based) sequence logo plots is returned. When a valid file name is specified, the list of plots is also written to the PDF file (one plot per page).

Examples

```r
res <- readRDS(system.file("extdata", "example_seqArchResult.rds", package = "seqArchR", mustWork = TRUE))

# Default position labels 1 to length of the sequences.
# Can also set pos_lab based on biology, e.g., use -50 to 49 denoting
# 50 basepairs upstream and 49 downstream of the transcription start site
# located at position 0.
arch_pl <- plot_arch_for_clusters(seqs = seqs_str(res),
    clust_list = res$clustSol$clusters,
    pos_lab = NULL,
    pdf_name = NULL,
    fixed_coord = TRUE)

# Using cowplot::plot_grid
arch_pl <- plot_arch_for_clusters(seqs = seqs_str(res),
    clust_list = res$clustSol$clusters,
    pos_lab = seq(100),
    method = "bits",
    pdf_name = NULL, show = FALSE)
cowplot::plot_grid(plotlist = arch_pl, ncol=1)

# Plotting architecture sequence logos with probability instead of
# information content
arch_pl <- plot_arch_for_clusters(seqs = seqs_str(res),
    clust_list = res$clustSol$clusters,
    pos_lab = seq(100),
    method = "prob",
    pdf_name = NULL, show = FALSE)
cowplot::plot_grid(plotlist = arch_pl, ncol=1)
```

---

**plot_ggseqlogo_of_seq**

*Plot sequence logo of a collection of sequences*

Description

A wrapper to ggseqlogo plotting. Given a collection of sequences, this function plots the sequence logo.
plot_ggseqlogo_of_seqs

Usage

plot_ggseqlogo_of_seqs(
  seqs,
  pos_lab = NULL,
  xt_freq = 5,
  method = "bits",
  title = NULL,
  bits_yax = "full",
  fixed_coord = FALSE
)

Arguments

seqs Collection of sequences as a DNAStringSet object.
pos_lab Labels for sequence positions, should be of same length as that of the sequences. Default value is NULL, when the positions are labeled from 1 to the length of the sequences.
xt_freq Specify the frequency of the x-axis ticks.
method Specify either 'bits' for information content or 'prob' for probability.
title The title for the plot. Default is NULL.
bits_yax Specify 'full' if the information content y-axis limits should be 0-2 or 'auto' for a suitable limit. The 'auto' setting adjusts the y-axis limits according to the maximum information content of the sequence logo. Default is 'full'.
fixed_coord Specify TRUE if the aspect ratio of the plot should be fixed, FALSE otherwise. Default is TRUE. When 'method' argument is set to 'bits', ratio is 4, when 'prob', ratio is 6.

Value

A sequence logo plot of the given DNA sequences.

See Also

plot_arch_for_clusters for obtaining multiple sequence logo plots as a list.

Examples

res <- readRDS(system.file("extdata", "example_seqArchRresult.rds", package = "seqArchR", mustWork = TRUE))

# Default, using information content on y-axis
pl <- plot_ggseqlogo_of_seqs(seqs = seqs_str(res, iter=1, cl=3),
  pos_lab = seq_len(100), title = NULL,
  fixed_coord = TRUE)

pl

# Using probability instead of information content
pl <- plot_ggseqlogo_of_seqs(seqs = seqs_str(res, iter=1, cl=3),
prepare_data_from_FASTA

Generate one-hot encoding of sequences given as FASTA file

Description
Given a set of sequences in a FASTA file this function returns a sparse matrix with one-hot encoded sequences. In this matrix, the sequence features are along rows, and sequences along columns. Currently, mono- and dinucleotide features for DNA sequences are supported. Therefore, the length of the feature vector is 4 and 16 times the length of the sequences (since the DNA alphabet is four characters) for mono- and dinucleotide features respectively.

Usage
prepare_data_from_FASTA(fasta_fname, raw_seq = FALSE, sinuc_or_dinuc = "sinuc")

Arguments
- fasta_fname: Provide the name (with complete path) of the input FASTA file.
- raw_seq: TRUE or FALSE, set this to TRUE if you want the raw sequences.
- sinuc_or_dinuc: character string, 'sinuc' or 'dinuc' to select for mono- or dinucleotide profiles.

Value
A sparse matrix of sequences represented with one-hot-encoding.

See Also
generate_one_hot_encoded_seqs for directly using a DNAStringSet object

Other input functions: generate_one_hot_encoded_seqs()

Examples
fname <- system.file("extdata", "example_data.fa.gz", 
                      package = "seqArchR", mustWork = TRUE)

# mononucleotides feature matrix
rawSeqs <- prepare_data_from_FASTA(fasta_fname = fname, 
                                   sinuc_or_dinuc = "sinuc")

# dinucleotides feature matrix
rawSeqs <- prepare_data_from_FASTA(fasta_fname = fname, 
                                   sinuc_or_dinuc = "dinuc")
# FASTA sequences as a Biostrings::DNAStringSet object
rawSeqs <- prepare_data_from_FASTA(fasta_fname = fname,
  raw_seq = TRUE)

---

**seqArchR**  

**seqArchR: A package for de novo discovery of different sequence architectures**

**Description**

Given a set of DNA sequences, seqArchR enables unsupervised discovery of \_de novo\_ clusters with characteristic sequence architectures characterized by position-specific motifs or composition of stretches of nucleotides, e.g., CG-richness, etc.

Call this function to process a data set using seqArchR.

**Usage**

```r
seqArchR(
  config,
  seqs_ohe_mat,
  seqs_raw,
  seqs_pos = NULL,
  total_itr = NULL,
  set_ocollation = NULL,
  fresh = TRUE,
  use_oc = NULL,
  o_dir = NULL
)
```

**Arguments**

- **config**: seqArchR configuration object as returned by `set_config`. This is a required argument.
- **seqs_ohe_mat**: A matrix of one-hot encoded sequences with sequences along columns. This is a required argument.
- **seqs_raw**: A DNAStringSet object. The FASTA sequences as a DNAStringSet object. This argument required argument.
- **seqs_pos**: Vector. Specify the tick labels for sequence positions. Default is NULL.
- **total_itr**: Numeric. Specify the number of iterations to perform. This should be greater than zero. Default is NULL.
- **set_ocollation**: Logical vector. A logical vector of length ‘total_itr’ specifying for every iteration of seqArchR if collation of clusters from outer chunks should be performed. TRUE denotes clusters are collated, FALSE otherwise.
Logical. Specify if this is (not) a fresh run. Because seqArchR enables checkpointing, it is possible to perform additional iterations upon clusters from an existing seqArchR result (or a checkpoint object). See ‘use_oc’ argument. For example, when processing a set of FASTA sequences, if an earlier call to seqArchR performed two iterations, and now you wish to perform a third, the arguments ‘fresh’ and ‘use_oc’ can be used. Simply set ‘fresh’ to FALSE and assign the sequence clusters from iteration two from the earlier result to ‘use_oc’. As of v0.1.3, with this setting, seqArchR returns a new result object as if the additional iteration performed is the only iteration.

List. Clusters to be further processed with seqArchR. These can be from a previous seqArchR result (in which case use get_seqs_clust_list function), or simply clusters from any other method. Warning: This has not been rigorously tested yet (v0.1.3).

Character. Specify the output directory with its path. seqArchR will create this directory. If a directory with the given name exists at the given location, seqArchR will add a suffix to the directory name. This change is reported to the user. Default is NULL. When NULL, just the result is returned, and no plots or checkpoints or result is written to disk.

Details

The seqArchR package provides three categories of important functions: related to data preparation and manipulation, performing non-negative matrix factorization, performing clustering, and visualization-related functions.

Value

A nested list of elements as follows:

- **seqsClustLabels**: A list with cluster labels for all sequences per iteration of seqArchR. The cluster labels as stored as characters.

- **clustBasisVectors**: A list with information on NMF basis vectors per iteration of seqArchR. Per iteration, there are two variables ‘nBasisVectors’ storing the number of basis vectors after model selection, and ‘basisVectors’, a matrix storing the basis vectors themselves. Dimensions of the ‘basisVectors’ matrix are 4*L x nBasisVectors (mononucleotide case) or 16*L x nBasisVectors (dinucleotide case).

- **clustSol**: The clustering solution obtained upon processing the raw clusters from the last iteration of seqArchR’s result. This is handled internally by the function collate_seqArchR_result using the default setting of Euclidean distance and ward.D linkage hierarchical clustering.

- **rawSeqs**: The input sequences as a DNAStringSet object.

- **timeInfo**: Stores the time taken (in minutes) for processing each iteration. This element is added only if ‘time’ flag is set to TRUE in config.

- **config**: The configuration used for processing.

- **call**: The function call itself.
Functions for data preparation and manipulation

- `prepare_data_from_FASTA`
- `get_one_hot_encoded_seqs`

Functions for visualizations

- `plot_arch_for_clusters`
- `plot_ggseqlogo_of_seqs`
- `viz_bas_vec`
- `viz_seqs_acgt_mat`
- `viz_pwm`

Examples

```r
# Here, we re-use the example input sequences and one-hot encoded matrix
# shipped with seqArchR. Please see examples in the corresponding man pages
# for generating a one-hot encoded input matrix from raw FASTA sequences
# in `prepare_data_from_FASTA`

inputSeqsMat <- readRDS(system.file("extdata", "tssSinuc.rds", package = "seqArchR", mustWork = TRUE))

inputSeqsRaw <- readRDS(system.file("extdata", "tssSeqsRaw.rds", package = "seqArchR", mustWork = TRUE))

# Set seqArchR configuration
seqArchRconfig <- seqArchR::set_config(
  parallelize = TRUE,
  n_cores = 2,
  n_runs = 100,
  k_min = 1,
  k_max = 20,
  mod_sel_type = "stability",
  bound = 10^-8,
  chunk_size = 100,
  flags = list(debug = FALSE, time = TRUE, verbose = TRUE, plot = FALSE)
)

# Run seqArchR
seqArchRresult <- seqArchR::seqArchR(config = seqArchRconfig,
  seqs_ohe_mat = inputSeqsMat,
  seqs_raw = inputSeqsRaw,
  seqs_pos = seq(1,100,by=1),
  total_itr = 2,
  set_ocollation = c(TRUE, FALSE))
```
seqs_str

Get sequences from the seqArchR result object

Description

Wrapper to fetch sequences from the seqArchR result object as character

Usage

```r
seqs_str(res, iter = NULL, cl = NULL, ord = FALSE)
```

Arguments

- `res`: seqArchR result object
- `iter`: Specify the iteration of seqArchR result. If set to NULL (the default), the original set of sequences (‘seqArchRresult$rawSeqs’) is returned.
- `cl`: Specify the cluster number. Sequences belonging to this cluster in iteration ‘iter’ of seqArchR result are returned as character. When ‘iter’ is NULL, this is treated as denoting the cluster number in seqArchR’s final clustering solution (‘seqArchRresult$clustSol$clusters’).
- `ord`: Specify TRUE if sequences are ordered by clusters. The original ordering of the sequences can be fetched by setting ‘iter’ to NULL and ‘ord’ to FALSE.

Details

Setting iter to NULL will fetch sequences as per the final clustering solution of seqArchR (‘clustSol$clusters’). When ‘iter’ is not NULL, use ‘cl’ to further choose a particular cluster. When ‘cl’ is NULL, the set of sequences returned can be ordered by clusters with ‘ord = TRUE’. Using ‘ord = FALSE’ fetches the sequences by their original order.

Value

The selected DNA sequences from the DNASTringSet object as a character vector.

Examples

```r
res <- system.file("extdata", "example_seqArchRresult.rds", package = "seqArchR", mustWork = TRUE)

# Fetch sequences from 2nd cluster of seqArchR's final solution
ans <- seqArchR::seqs_str(readRDS(res), iter=NULL, cl=2)

# Fetch all sequences ordered by the final clustering
ans <- seqArchR::seqs_str(readRDS(res), iter=NULL, cl=NULL, ord=TRUE)

# Fetch sequences belonging to first cluster in seqArchR's first iteration
ans <- seqArchR::seqs_str(readRDS(res), iter=1, cl=1)
```
set_config

Set seqArchR run configuration

Description

This function sets the configuration for `seqArchR`.

Usage

```r
set_config(
    chunk_size = 500,
    k_min = 1,
    k_max = 50,
    mod_sel_type = "stability",
    bound = 1e-6,
    cv_folds = 5,
    parallelize = FALSE,
    n_cores = NA,
    n_runs = 100,
    alpha_base = 0,
    alpha_pow = 1,
    min_size = 25,
    result_aggl = "complete",
    result_dist = "euclid",
    checkpointing = TRUE,
    flags = list(debug = FALSE, time = FALSE, verbose = TRUE, plot = FALSE)
)
```

Arguments

- `chunk_size` Numeric. Specify the size of the inner chunks of sequences.
- `k_min` Numeric. Specify the minimum of the range of values to be tested for number of NMF basis vectors. Default is 1.
- `k_max` Numeric. Specify the maximum of the range of values to be tested for number of NMF basis vectors. Default is 50.
- `mod_sel_type` Character. Specify the model selection strategy to be used. Default is `stability`. Another option is `cv`, short for cross-validation. Warning: The cross-validation approach can be time consuming and computationally expensive than the stability-based approach.
- `bound` Numeric. Specify the lower bound value as criterion for choosing the most appropriate number of NMF factors. Default is 1e-08.
- `cv_folds` Numeric. Specify the number of cross-validation folds used for model selection. Only used when `mod_sel_type` is set to `cv`. Default value is 5.

parallelize Logical. Specify whether to parallelize the procedure. Note that running seqArchR serially can be time consuming, especially when using cross-validation for model selection. See ‘n_cores’. Consider parallelizing with at least 2 or 4 cores.

n_cores The number of cores to be used when ‘parallelize’ is set to TRUE. If ‘parallelize’ is FALSE, nCores is ignored.

n_runs Numeric. Specify the number of bootstrapped runs to be performed with NMF. Default value is 100. When using cross-validation more than 100 iterations may be needed (up to 500).

alpha_base, alpha_pow Specify the base and the power for computing ‘alpha’ in performing model selection for NMF. alpha = alpha_base^alpha_pow. Alpha specifies the regularization for NMF. Default: 0 and 1 respectively. _Warning_: Currently, not used (for future).

min_size Numeric. Specify the minimum number of sequences, such that any cluster/chunk of size less than or equal to it will not be further processed. Default is 25.

result_aggl Character. Specify the agglomeration method to be used for final result collation with hierarchical clustering. Default is ‘complete’ linkage. Possible values are those allowed with hclust. Also see details below.

result_dist Character. Specify the distance method to be used for final result collation with hierarchical clustering. Default is ‘cor’ for correlation. Possible values are those allowed with hclust. Also see details below.

checkpointing Logical. Specify whether to write intermediate checkpoints to disk as RDS files. Checkpoints and the final result are saved to disk provided the ‘o_dir’ argument is set in seqArchR. When ‘o_dir’ argument is not provided or NULL, this is ignored. Default is TRUE.

flags List with four logical elements as detailed.

default Whether debug information for the run is printed
verbose Whether verbose information for the run is printed
plot Whether verbose plotting is performed for the run
time Whether timing information is printed for the run

Details Setting suitable values for the following parameters is dependent on the data: ‘inner_chunk_size’, ‘k_min’, ‘k_max’, ‘mod_sel_type’, ‘min_size’, ‘result_aggl’, ‘result_dist’.

Value A list with all params for seqArchR set

Examples

# Set seqArchR configuration
seqArchRconfig <- seqArchR::set_config(chunk_size = 100,
parallelize = TRUE,
n_cores = 2,
n_runs = 100,
k_min = 1,
k_max = 20,
mod_sel_type = "stability",
bound = 10^-8,
flags = list(debug = FALSE, time = TRUE, verbose = TRUE,
plot = FALSE)
)

viz_bas_vec

Visualize the NMF basis vectors

Description
The given features matrix is visualized as a paired heatmap and sequence logo where the positions
are aligned for better visualization, or as a single heatmap or as a single sequence logo.

Usage

viz_bas_vec(
  feat_mat,
  ptype = c("heatmap", "seqlogo"),
  method = "bits",
  pos_lab = NULL,
  pdf_name = NULL,
  add_pseudo_counts = FALSE,
  sinuc_or_dinuc = "sinuc",
  fixed_coord = FALSE
)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>feat_mat</td>
<td>The features matrix (basis vectors matrix) from seqArchR.</td>
</tr>
<tr>
<td>ptype</td>
<td>Character vector of length one or two. Specify just one of &quot;heatmap&quot; or &quot;seqlogo&quot; to visualize the basis vectors as such, or specify a vector of length two for plotting both, heatmap and seqlogo. These are then arranged one below the other, the first on top and the second under it.</td>
</tr>
<tr>
<td>method</td>
<td>Specify either of &quot;custom&quot;, &quot;bits&quot;, or &quot;probability&quot; for plotting sequence logo. Default is &quot;bits&quot;.</td>
</tr>
<tr>
<td>pos_lab</td>
<td>Labels for sequence positions, should be of same length as that of the sequences. Default value is NULL, when the positions are labeled from 1 to the length of the sequences.</td>
</tr>
<tr>
<td>pdf_name</td>
<td>Filename to save the plot, also provide the extension.</td>
</tr>
</tbody>
</table>
add_pseudo_counts
Logical, taking values TRUE or FALSE, default set to FALSE. Setting it to TRUE will enable adding pseudo-counts to the features matrix.

sinuc_or_dinuc
"sinuc" or "dinuc" for choosing between mono- and dinucleotide profiles respectively.

fixed_coord
Set this to TRUE to use a fixed aspect ratio for the plot irrespective of the width and height of the PDF. Default is FALSE.

Value
nothing

See Also
Other visualization functions: viz_pwm(), viz_seqss_acgt_mat()

Examples
res <- readRDS(system.file("extdata", "example_seqArchRresult.rds", package = "seqArchR", mustWork = TRUE))

# Visualize basis vectors at iteration 1 of seqArchR result as heatmap and sequence logo
viz_bas_vec(feat_mat = get_clBasVec_m(res, iter=1), sinuc_or_dinuc = "dinuc", ptype = c("heatmap", "seqlogo"))

# Visualize basis vectors at iteration 1 of seqArchR result as sequence logos
viz_bas_vec(feat_mat = get_clBasVec_m(res, iter=1), ptype = "seqlogo", sinuc_or_dinuc = "dinuc")

# Visualizing basis vector for a single cluster as a heatmap
viz_bas_vec(feat_mat = as.matrix(get_clBasVec_m(res, iter=1)[[,3]], ptype = "heatmap", sinuc_or_dinuc = "dinuc")

viz_pwm
Visualize a position weight matrix as a heatmap or sequence logo

Description
The given position weight matrix is plotted as a heatmap or sequence logo
Usage

```r
viz_pwm(
  pwm_mat,
  method = "heatmap",
  pos_lab = NULL,
  pdf_name = NULL,
  fixed_coord = FALSE,
  bits_yax = "full"
)
```

Arguments

- `pwm_mat`: Matrix (usually a PWM, but can be any non-normalized matrix) to be visualized. Rownames must be letters.
- `method`: Character. Set this to 'heatmap' when plotting a heatmap, else you can set it to either of 'custom', 'bits', or 'probability' when you wish to visualize it as a sequence logo. Default is 'heatmap'.
- `pos_lab`: Labels for sequence positions, should be of same length as that of the sequences. Default value is NULL, when the positions are labeled from 1 to the length of the sequences.
- `pdf_name`: Name of the file which will be saved as PDF.
- `fixed_coord`: Set this to TRUE to use a fixed aspect ratio for the plot. Default is FALSE.
- `bits_yax`: Specify 'full' if the information content y-axis limits should be 0-2 or 'auto' for a suitable limit. The 'auto' setting adjusts the y-axis limits according to the maximum information content of the sequence logo. Default is 'full'.

Value

A ggplot object so you can simply call print or save on it later. If pdf_name is given, it is also saved and the ggplot2 object returned.

See Also

- `plot_ggseqlogo_of_seqs` for visualizing a collection of sequences by their sequence logo.
- Other visualization functions: `viz_bas_vec()`, `viz_seqs_acgt_mat()`

Examples

```r
res <- readRDS(system.file("extdata", "example_seqArchRresult.rds", package = "seqArchR", mustWork = TRUE))

pwm <- seqArchR::make_PWMs(get_clBasVec_m(res, iter=1)[,1],
                          add_pseudo_counts = FALSE, sinuc = FALSE)

viz_pwm(pwm_mat = pwm, method = "heatmap", fixed_coord = TRUE)

viz_pwm(pwm_mat = pwm, method = "bits", fixed_coord = TRUE)
```
viz_seqs_acgt_mat

Visualize raw DNA sequences as an image

**Description**

This function plots the collection of sequences as an image matrix.

**Usage**

```r
text = "viz_seqs_acgt_mat(
  seqs,
  pos_lab = NULL,
  xt_freq = min(length(pos_lab), 5),
  yt_freq = min(length(seqs), 100),
  use_col = c("darkgreen", "blue", "orange", "red"),
  add_legend = TRUE,
  use_legend = Biostrings::DNA_BASES,
  save_fname = NULL,
  file_type = "PNG",
  f_width = 450,
  f_height = 900,
  f_units = "px"
)
```

**Arguments**

- `seqs` The sequences as a DNAStringSet object.
- `pos_lab` The labels to be used for the sequence positions. Default: Sequence positions are labeled from 1 to the length of the sequences.
- `xt_freq` The x-axis tick frequency. Expects a positive integer less than the length of the sequences. Default is 5.
- `yt_freq` The y-axis tick frequency. Expects a positive integer less than number of sequences. Default is 100.
- `use_col` A vector of four colors used for the DNA bases A, C, G, and T (in that order).
- `add_legend` Logical. Whether legend should be added to the plot. Default is TRUE.
- `use_legend` A character vector of letters in the input sequences. Default is DNA_BASES, used for DNA sequences.
- `save_fname` Specify the filename (with extension) for saving the plot to disk.
- `file_type` Specify the file type, namely PNG, JPEG, TIFF.
- `f_width` Specify the width for the plot. This depends on the length of sequences.
- `f_height` Specify the height for the plot. This depends on the number of sequences.
- `f_units` Specify the units in which the height and width are given.
Value

Nothing returned to the R interpreter.

See Also

Other visualization functions: \texttt{viz\_bas\_vec()}, \texttt{viz\_pwm()}

Examples

```r
res <- readRDS(system.file("extdata", "example_seqArchRresult.rds", package = "seqArchR", mustWork = TRUE))

# Image matrix of sequences in the input order
viz\_seqs\_acgt\_mat(seqs = seqs\_str(res))

# Image matrix of sequences ordered by the clustering from seqArchR
use\_seqs <- seqs\_str(res, iter = NULL, cl = NULL, ord = TRUE)
viz\_seqs\_acgt\_mat(seqs = use\_seqs)

# Image matrix of sequences belonging to a single cluster
use\_seqs <- seqs\_str(res, iter = 2, cl = 2)
viz\_seqs\_acgt\_mat(seqs = use\_seqs)
```
Index

* input functions
  get_one_hot_encoded_seqs, 6
  prepare_data_from_FASTA, 12
* visualization functions
  viz_bas_vec, 19
  viz_pwm, 20
  viz_seqs_acgt_mat, 22

collate_clusters, 2
collate_seqArchR_result, 3, 14

DNA_BASES, 22
DNAStringSet, 6, 9, 11, 13

get_clBasVec, 5
get_clBasVec_k (get_clBasVec), 5
get_clBasVec_m (get_clBasVec), 5
get_one_hot_encoded_seqs, 6, 12, 15
get_seqClLab (get_clBasVec), 5
get_seqs_clust_list, 7, 14

hclust, 4, 18

make_PWMs, 8

plot_arch_for_clusters, 9, 11, 15
plot_ggseqlogo_of_seqs, 9, 10, 15, 21
prepare_data_from_FASTA, 7, 12, 15

seqArchR, 13, 18
seqs_str, 6, 16
set_config, 13, 17

viz_bas_vec, 15, 19, 21, 23
viz_pwm, 15, 20, 20, 23
viz_seqs_acgt_mat, 15, 20, 21, 22