Package 'iimi'

July 26, 2024

Title Identifying Infection with Machine Intelligence

Date/Publication 2024-07-26 08:20:02 UTC

Version 1.1.1

Description A novel machine learning method for plant viruses diagnostic using genome sequencing data. This package includes three different machine learning models, random forest, XGBoost, and elastic net, to train and predict mapped genome samples. Mappability profile and unreliable regions are introduced to the algorithm, and users can build a mappability profile from scratch with functions included in the package. Plotting mapped sample coverage information is provided.

```
Encoding UTF-8
RoxygenNote 7.3.1
LazyData true
VignetteBuilder knitr
Imports GenomicAlignments, IRanges, Rsamtools, data.table, mltools,
      randomForest, xgboost, Biostrings, stats, MTPS, R.utils, caret,
      stringr, dplyr, Rdpack
RdMacros Rdpack
Depends R (>= 3.5.0)
Suggests testthat (>= 3.0.0), knitr, rmarkdown, httr
Config/testthat/edition 3
License MIT + file LICENSE
LazyDataCompression xz
NeedsCompilation no
Author Haochen Ning [aut],
      Ian Boyes [aut],
      Ibrahim Numanagić [aut] (<a href="https://orcid.org/0000-0002-2970-7937">https://orcid.org/0000-0002-2970-7937</a>),
      Michael Rott [aut],
      Li Xing [aut] (<a href="https://orcid.org/0000-0002-4186-7909">https://orcid.org/0000-0002-4186-7909</a>),
      Xuekui Zhang [aut, cre] (<a href="https://orcid.org/0000-0003-4728-2343">https://orcid.org/0000-0003-4728-2343</a>)
Maintainer Xuekui Zhang <xuekui@uvic.ca>
Repository CRAN
```

2 convert_bam_to_rle

Contents

convert_bam_to_rle	2
convert_rle_to_df	3
create_high_nucleotide_content	4
	4
	5
	6
nucleotide_info	6
plot_cov	7
predict_iimi	8
trained_xgb	9
unreliable_regions	11
virus_segments	11
1	13
ert_bam_to_rle	_
•	convert_rle_to_df create_high_nucleotide_content create_mappability_profile example_cov example_diag nucleotide_info plot_cov predict_iimi trained_en trained_rf trained_xgb train_iimi unreliable_regions virus_segments

Description

Converts one or more indexed and sorted BAM files into a run-length encodings (RLEs) list.

Usage

```
convert_bam_to_rle(bam_file, paired = FALSE)
```

Arguments

bam_file path to BAM file(s).

paired Indicate if the sequencing paired is single-end or paired-end reads. TRUE if

paired-end. FALSE if single-end.

Value

A list of coverage profile(s) in RLE format with one or more samples.

```
## Not run:
## Please change the path to your folder where you
## store sorted and indexed BAM files of mapped samples
rles <- convert_bam_to_rle("path/to/bam/file")</pre>
```

convert_rle_to_df 3

```
## End(Not run)
```

convert_rle_to_df convert_rle_to_df

Description

Converts a list of run-length encodings (RLEs) into a data frame with 16 features after mappability profiling and nucleotide filtering.

Usage

```
convert_rle_to_df(
  covs,
  unreliable_region_df = unreliable_regions,
  unreliable_region_enabled = TRUE,
  additional_nucleotide_info = data.frame()
)
```

Arguments

covs A list of Coverage profile(s) in RLE format. Can be one or more samples. $unreliable_region_df$

The unreliable regions of the virus segments. Default is unreliable_regions. It includes the mappability profile from a host genome (we only have Arabidopsis thaliana right now) and virus references, and the regions that have CG% and A% over 60% and 45% respectively.

unreliable_region_enabled

Default is TRUE. If TRUE, the input will be checked against unreliable_region_df. If FALSE, this step will be skipped.

additional_nucleotide_info

Additional nucleotide information for virus segments that are not included in nucleotide_info. The information provided must be a data frame that follows the format of nucleotide_info. Default is an empty data frame.

Value

A data frame object that contains the mapping result for each virus segment that the plant sample reads are aligned to and a RLE list of coverage information.

```
## Not run:
df <- convert_rle_to_df(example_cov)
## End(Not run)</pre>
```

Description

Creates a data frame of the start and end positions of the regions_a that are considered high in A% and GC%.

Usage

```
create_high_nucleotide_content(gc = 0.6, a = 0.45, window = 75)
```

Arguments

gc	The threshold for GC content. It is the proportion of G and C nucleotides in a sliding window. Default is 0.6.
a	The threshold for A nucleotide. It is the proportion of A nucleotide in a sliding window. Default is 0.45.
window	The sliding window size of your choice. Default is 75.

Value

A data frame of the start and end positions of the regions_a that are considered high in A% and GC%.

Examples

```
## Not run: high_nucleotides_regions <- create_high_nucleotide_content()</pre>
```

Description

Creates a data frame of start and end positions of the regions that are considered unmappable. Unmappable areas indicate that they can be mapped to another virus segment or a host genome. Note that we only have Arabidopsis Thaliana as a host.

Usage

```
create_mappability_profile(path_to_bam_files, category, window = 75)
```

example_cov 5

Arguments

path_to_bam_files

Path to the folder that stores the indexed and sorted BAM file(s).

category Type of unreliable region you are creating. You can use categories in the pro-

vided unreliable_regions data frame or customize in your own way.

window The sliding window size of your choice. Default is 75.

Value

A data frame of start and end positions of the regions that are considered unmappable.

Examples

```
## Not run:
## Please change the path to your folder where you store the mapped viruses
mappability_profile <- create_mappability_profile("path/to/folder",
    category = "Unmappable regions")
## End(Not run)</pre>
```

example_cov

Coverage profiles of three plant samples.

Description

A list of coverage profiles for three plant samples. This is only a toy sample. You can use it for running the examples in the vignette. We recommend using more data to train the model, the more the better.

Usage

```
example_cov
```

Format

A list of 3 run length encoding (RLE) lists for 3 plant samples. Each RLE list has the RLE vector of a virus segment

nucleotide_info

example_diag

Known diagnostics result of virus segments

Description

A matrix containing the known truth about the diagnostics result for each plant sample for the example data. It records whether the sample is infected with a virus segment. Each column is a sample, and each row is a virus segment's diagnostics status for three samples.

Usage

example_diag

Format

A matrix with 3 columns:

- S1 Sample one
- S2 Sample two
- S3 Sample three

nucleotide_info

Nucleotide information of virus segments

Description

A data set containing the GC content and other information about the virus segments from the official Virtool virus data base (version 1.4.0). The variables are as follows:

Usage

```
nucleotide_info
```

Format

A data frame with 7 variables:

virus_name The virus name

iso_id The virus isolate ID

seg_id The virus segment ID

A_percent The percentage of A nucleotides in the virus segment

C_percent The percentage of C nucleotides in the virus segment

T_percent The percentage of T nucleotides in the virus segment

GC_percent The percentage of G and C nucleotides in the virus segment (GC content)

seg_len The length of the virus segment

plot_cov 7

plot_cov()

Description

Plots the coverage profile of the mapped plant sample.

Usage

```
plot_cov(
   covs,
   legend_status = TRUE,
   nucleotide_status = TRUE,
   window = 75,
   ...
)
```

Arguments

covs An RLE list of coverage information of one or more plant samples.

legend_status Whether display legend. Default is TRUE.

nucleotide_status
Whether display a sliding window of A percentage and CG content. Default is TRUE.

window The sliding window size. Default is 75.

Other arguments that can be passed to plot, lines, or legend.

Value

The coverage profile of the mapped plant sample.

```
plot_cov(example_cov$S1)
```

8 predict_iimi

redict_iimi	predict_iimi()

Description

Uses a machine learning model to predict the infection status for the plant sample(s). User can use their own model if needed.

Usage

```
predict_iimi(newdata, method = "xgb", trained_model, report_virus_level = TRUE)
```

Arguments

newdata A matrix or data frame that contains the features extracted from the coverage

profile using convert_bam_to_cov().

method The machine learning method of choice, rf, xgb, or en. rf stands for ran-

dom forest model; xgb stands for XGBoost model; and en stands for elastic net

model.

trained_model The trained model. If not provided, default model is used.

report_virus_level

If TRUE, the function returns the aggregated results based on the virus. If FALSE, the function returns the unaggregated results based on segment level with each decision's probability decided by the model. We do not recommended to set this to FALSE.

Value

A data frame of diagnostics result for each sample

```
## Not run: df <- convert_rle_to_df(example_cov)
predictions <- predict_iimi(df)
## End(Not run)</pre>
```

trained_en 9

trained_en

A trained model using the default Elastic Net settings

Description

A trained model using the default Elastic Net settings

Usage

trained_en

Format

An object of class cv.glmnet of length 13.

trained_rf

A trained model using the default Random Forest settings

Description

A trained model using the default Random Forest settings

Usage

trained_rf

Format

An object of class randomForest. formula (inherits from randomForest) of length 15.

trained_xgb

A trained model using the default XGBoost settings

Description

A trained model using the default XGBoost settings

Usage

trained_xgb

Format

An object of class list of length 2.

10 train_iimi

Description

Trains a XGBoost (default), Random Forest, or Elastic Net model using user-provided data.

Usage

```
train_iimi(
   train_x,
   train_y,
   method = "xgb",
   nrounds = 100,
   max_depth = 10,
   gamma = 6,
   ntree = 100,
   k = 5,
   ...
)
```

Arguments

A data frame or a matrix of predictors. train_x A response vector of labels (needs to be a factor). train_y The machine learning method of choice, Random Forest or XGBoost, or Elastic Net method model. Default is XGBoost model. Max number of boosting iterations for XGBoost model. Default is 100. nrounds Maximum depth of a tree in XGBoost model. Default is 10. max_depth Minimum loss reduction required in XGBoost model. Default is 6. gamma Number of trees in Random Forest model. Default is 100. ntree k Number of folds. Default is 5. Other arguments that can be passed to randomForest, xgboost, or glmnet.

Value

A Random Forest, XGBoost, Elastic Net model

```
## Not run:
df <- convert_rle_to_df(example_cov)
train_x <- df[,-c(1:4)]
train_y = c()
for (ii in 1:nrow(df)) {</pre>
```

unreliable_regions 11

```
seg_id = df$seg_id[ii]
sample_id = df$sample_id[ii]
train_y = c(train_y, example_diag[seg_id, sample_id])
}
trained_model <- train_iimi(train_x = train_x, train_y = train_y)
## End(Not run)</pre>
```

unreliable_regions

The unreliable regions of the virus segments

Description

A data frame of unmappable regions and regions of CG% and A% over 60% and 45% respectively for the virus segments. It is worth to note that if a virus segment does not have any unreliable regions, that virus segment is not shown in this data frame.

Usage

```
unreliable_regions
```

Format

A data frame of unreliable regions in the run-length encoding format for virus segments.

Start The start position of the region that is considered unreliable

End The end position of the region that is considered unreliable

Virus segment The virus segment ID

Categories The category that this unrelible region belong to, which are Unmappable regions (host), Unmappable regions (virus), CG% > 60%, A% > 45%.

virus_segments

A DNAStringSet of virus segments from the Virtool virus data base (version 1.4.0)

Description

A DNAStringSet of virus segments from the Virtool virus data base (version 1.4.0)

Usage

```
virus_segments
```

virus_segments

Format

An object of class DNAStringSet of length 3138.

Index

```
* datasets
    example_cov, 5
     example_diag, 6
     nucleotide\_info, 6
     trained_en,9
     trained_rf, 9
     trained_xgb, 9
     unreliable\_regions, 11
     virus_segments, 11
convert_bam_to_rle, 2
convert_rle_to_df, 3
\verb|create_high_nucleotide_content|, 4
create_mappability_profile, 4
example_cov, 5
\texttt{example\_diag}, \textcolor{red}{6}
nucleotide_info, 6
plot_cov, 7
\verb|predict_iimi|, 8
train_iimi, 10
{\tt trained\_en}, \textcolor{red}{9}
trained_rf, 9
trained_xgb, 9
unreliable\_regions, 11
\textit{virus\_segments}, 11
```