Package 'seqtrie'

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Title Radix Tree and Trie-Based String Distances

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Description A collection of Radix Tree and Trie algorithms for finding similar sequences and calculating sequence distances (Levenshtein and other distance metrics). This work was inspired by a trie implementation in Python: ``Fast and Easy Levenshtein distance using a Trie." Hanov (2011) <http://stevehanov.ca/blog/index.php?id=114>.

License GPL-3

Biarch true

Encoding UTF-8

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LazyData true

SystemRequirements GNU make

LinkingTo Rcpp, RcppParallel, BH

- Imports Rcpp (>= 0.12.18.3), RcppParallel (>= 5.1.3), R6, rlang, dplyr, stringi
- **Suggests** knitr, rmarkdown, stringdist, qs, Biostrings, pwalign, igraph, ggplot2

VignetteBuilder knitr

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Copyright This package includes code from the 'span-lite' library owned by Martin Moene under Boost Software License 1.0. This package includes code from the 'ankerl' library owned by Martin Leitner-Ankerl under MIT License. This package contains data derived from Adaptive Biotechnologies ``ImmuneCODE'' dataset under Creative Commons Attribution 4.0.

URL https://github.com/traversc/seqtrie

BugReports https://github.com/traversc/seqtrie/issues NeedsCompilation yes Author Travers Ching [aut, cre, cph], Martin Moene [ctb, cph] (span-lite C++ library), Steve Hanov [ctb] (Trie levenshtein implementation in Python), Martin Leitner-Ankerl [ctb] (Ankerl unordered dense hashmap)

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covid_cdr3

Adaptive COVID TCRB CDR3 data

Description

Unique TCRB CDR3 sequences from the Nolan et al. 2020. CDR3s were extracted via IgBLAST. The license for this data is Creative Commons Attribution 4.0 International License.

Usage

data(covid_cdr3)

Format

A character vector of length 133,034.

References

Nolan, Sean, et al. "A large-scale database of T-cell receptor beta (TCRB) sequences and binding associations from natural and synthetic exposure to SARS-CoV-2." (2020). doi: 10.21203/rs.3.rs-51964/v1.

dist_matrix

Examples

```
data(covid_cdr3)
# Average CDR3 length
mean(nchar(covid_cdr3)) # [1] 43.56821
```

dist_matrix

Compute distances between all combinations of two sets of sequences

Description

Compute distances between all combinations of query and target sequences

Usage

```
dist_matrix(
  query,
  target,
  mode,
  cost_matrix = NULL,
  gap_cost = NULL,
  gap_open_cost = NULL,
  nthreads = 1,
  show_progress = FALSE
)
```

Arguments

query	A character vector of query sequences.
target	A character vector of target sequences.
mode	The distance metric to use. One of hamming (hm), global (gb) or anchored (an).
cost_matrix	A custom cost matrix for use with the "global" or "anchored" distance metrics. See details.
gap_cost	The cost of a gap for use with the "global" or "anchored" distance metrics. See details.
gap_open_cost	The cost of a gap opening. See details.
nthreads	The number of threads to use for parallel computation.
show_progress	Whether to show a progress bar.

Details

This function calculates all combinations of pairwise distances based on Hamming, Levenshtein or Anchored algorithms. The output is a NxM matrix where N = length(query) and M = length(target). Note: this can take a *really* long time; be careful with input size.

Three types of distance metrics are supported, based on the form of alignment performed. These are: Hamming, Global (Levenshtein) and Anchored.

An anchored alignment is a form of semi-global alignment, where the query sequence is "anchored" (global) to the beginning of both the query and target sequences, but is semi-global in that the end of the either the query sequence or target sequence (but not both) can be unaligned. This type of alignment is sometimes called an "extension" alignment in literature.

In contrast a global alignment must align the entire query and target sequences. When mismatch and indel costs are equal to 1, this is also known as the Levenshtein distance.

By default, if mode == "global" or "anchored", all mismatches and indels are given a cost of 1. However, you can define your own distance metric by setting the cost_matrix and gap parameters. The cost_matrix is a strictly positive square integer matrix and should include all characters in query and target as column- and rownames. To set the cost of a gap (insertion or deletion) you can include a row and column named "gap" in the cost_matrix *OR* set the gap_cost parameter (a single positive integer). Similarly, the affine gap alignment can be set by including a row and column named "gap_open" in the cost_matrix *OR* setting the gap_open_cost parameter (a single positive integer). If affine alignment is used, the cost of a gap is defined as: TOTAL_GAP_COST = gap_open_cost + (gap_cost * gap_length).

If mode == "hamming" all alignment parameters are ignored; mismatch is given a distance of 1 and gaps are not allowed.

Value

The output is a distance matrix between all query (rows) and target (columns) sequences. For anchored searches, the output also includes attributes "query_size" and "target_size" which are matrices containing the lengths of the query and target sequences that are aligned.

Examples

```
dist_matrix(c("ACGT", "AAAA"), c("ACG", "ACGT"), mode = "global")
```

dist_pairwise

Pairwise distance between two sets of sequences

Description

Compute the pairwise distance between two sets of sequences

dist_pairwise

Usage

```
dist_pairwise(
  query,
  target,
  mode,
  cost_matrix = NULL,
  gap_cost = NULL,
  gap_open_cost = NULL,
  nthreads = 1,
  show_progress = FALSE
)
```

Arguments

query	A character vector of query sequences.
target	A character vector of target sequences Must be the same length as query.
mode	The distance metric to use. One of hamming (hm), global (gb) or anchored (an).
cost_matrix	A custom cost matrix for use with the "global" or "anchored" distance metrics. See details.
gap_cost	The cost of a gap for use with the "global" or "anchored" distance metrics. See details.
gap_open_cost	The cost of a gap opening. See details.
nthreads	The number of threads to use for parallel computation.
show_progress	Whether to show a progress bar.

Details

This function calculates pairwise distances based on Hamming, Levenshtein or Anchored algorithms. *query* and *target* must be the same length.

Three types of distance metrics are supported, based on the form of alignment performed. These are: Hamming, Global (Levenshtein) and Anchored.

An anchored alignment is a form of semi-global alignment, where the query sequence is "anchored" (global) to the beginning of both the query and target sequences, but is semi-global in that the end of the either the query sequence or target sequence (but not both) can be unaligned. This type of alignment is sometimes called an "extension" alignment in literature.

In contrast a global alignment must align the entire query and target sequences. When mismatch and indel costs are equal to 1, this is also known as the Levenshtein distance.

By default, if mode == "global" or "anchored", all mismatches and indels are given a cost of 1. However, you can define your own distance metric by setting the cost_matrix and gap parameters. The cost_matrix is a strictly positive square integer matrix and should include all characters in query and target as column- and rownames. To set the cost of a gap (insertion or deletion) you can include a row and column named "gap" in the cost_matrix OR set the gap_cost parameter (a single positive integer). Similarly, the affine gap alignment can be set by including a row and column named "gap_open" in the cost_matrix OR setting the gap_open_cost parameter (a single positive integer). If affine alignment is used, the cost of a gap is defined as: TOTAL_GAP_COST = gap_open_cost + (gap_cost * gap_length).

If mode == "hamming" all alignment parameters are ignored; mismatch is given a distance of 1 and gaps are not allowed.

Value

The output of this function is a vector of distances. If mode == "anchored" then the output also includes attributes "query_size" and "target_size" which are vectors containing the lengths of the query and target sequences that are aligned.

Examples

```
dist_pairwise(c("ACGT", "AAAA"), c("ACG", "ACGT"), mode = "global")
```

dist_search

Distance search for similar sequences

Description

Find similar sequences within a distance threshold

Usage

```
dist_search(
  query,
  target,
  max_distance = NULL,
  max_fraction = NULL,
  mode = "levenshtein",
   cost_matrix = NULL,
  gap_cost = NULL,
  gap_open_cost = NULL,
  tree_class = "RadixTree",
  nthreads = 1,
  show_progress = FALSE
```

)

Arguments

query	A character vector of query sequences.
target	A character vector of target sequences.
<pre>max_distance</pre>	how far to search in units of absolute distance. Can be a single value or a vector. Mutually exclusive with max_fraction.
<pre>max_fraction</pre>	how far to search in units of relative distance to each query sequence length. Can be a single value or a vector. Mutually exclusive with max_distance.

dist_search

mode	The distance metric to use. One of hamming (hm), global (gb) or anchored (an).
cost_matrix	A custom cost matrix for use with the "global" or "anchored" distance metrics. See details.
gap_cost	The cost of a gap for use with the "global" or "anchored" distance metrics. See details.
gap_open_cost	The cost of a gap opening. See details.
tree_class	Which R6 class to use. Either RadixTree or RadixForest (default: RadixTree)
nthreads	The number of threads to use for parallel computation.
show_progress	Whether to show a progress bar.

Details

This function finds all sequences in *target* that are within a distance threshold of any sequence in *query*. This function uses either a RadixTree or RadixForest to store *target* sequences. See the R6 class documentation for additional details.

Three types of distance metrics are supported, based on the form of alignment performed. These are: Hamming, Global (Levenshtein) and Anchored.

An anchored alignment is a form of semi-global alignment, where the query sequence is "anchored" (global) to the beginning of both the query and target sequences, but is semi-global in that the end of the either the query sequence or target sequence (but not both) can be unaligned. This type of alignment is sometimes called an "extension" alignment in literature.

In contrast a global alignment must align the entire query and target sequences. When mismatch and indel costs are equal to 1, this is also known as the Levenshtein distance.

By default, if mode == "global" or "anchored", all mismatches and indels are given a cost of 1. However, you can define your own distance metric by setting the cost_matrix and gap parameters. The cost_matrix is a strictly positive square integer matrix and should include all characters in query and target as column- and rownames. To set the cost of a gap (insertion or deletion) you can include a row and column named "gap" in the cost_matrix *OR* set the gap_cost parameter (a single positive integer). Similarly, the affine gap alignment can be set by including a row and column named "gap_open" in the cost_of a gap is defined as: TOTAL_GAP_COST = gap_open_cost + (gap_cost * gap_length).

If mode == "hamming" all alignment parameters are ignored; mismatch is given a distance of 1 and gaps are not allowed.

Value

The output is a data.frame of all matches with columns "query" and "target". For anchored searches, the output also includes attributes "query_size" and "target_size" which are vectors containing the portion of the query and target sequences that are aligned.

```
dist_search(c("ACGT", "AAAA"), c("ACG", "ACGT"), max_distance = 1, mode = "levenshtein")
```

generate_cost_matrix Generate a simple cost matrix

Description

Generate a cost matrix for use with the search method

Usage

```
generate_cost_matrix(
   charset,
   match = 0L,
   mismatch = 1L,
   gap = NULL,
   gap_open = NULL
)
```

Arguments

charset	A string representing all possible characters in both query and target sequences (e.g. "ACGT")
match	The cost of a match
mismatch	The cost of a mismatch
gap	The cost of a gap or NULL if this parameter will be set later.
gap_open	The cost of a gap opening or NULL. If this parameter is set, gap must also be set.

Value

A cost matrix

Examples

```
generate_cost_matrix("ACGT", match = 0, mismatch = 1)
```

RadixForest

RadixForest

Description

Radix Forest class implementation

RadixForest

Details

The RadixForest class is a specialization of the RadixTree implementation. Instead of putting sequences into a single tree, the RadixForest class puts sequences into separate trees based on sequence length. This allows for faster searching of similar sequences based on Hamming or Levenshtein distance metrics. Unlike the RadixTree class, the RadixForest class does not support anchored searches or a custom cost matrix. See *RadixTree* for additional details.

Public fields

forest_pointer Map of sequence length to RadixTree

char_counter_pointer Character count data for the purpose of validating input

Methods

Public methods:

- RadixForest\$new()
- RadixForest\$show()
- RadixForest\$to_string()
- RadixForest\$graph()
- RadixForest\$to_vector()
- RadixForest\$size()
- RadixForest\$insert()
- RadixForest\$erase()
- RadixForest\$find()
- RadixForest\$prefix_search()
- RadixForest\$search()
- RadixForest\$validate()

Method new(): Create a new RadixForest object

Usage:

```
RadixForest$new(sequences = NULL)
```

Arguments:

sequences A character vector of sequences to insert into the forest

Method show(): Print the forest to screen

Usage: RadixForest\$show()

Method to_string(): Print the forest to a string

Usage: RadixForest\$to_string()

Method graph(): Plot of the forest using igraph

Usage:

RadixForest\$graph(depth = -1, root_label = "root", plot = TRUE)

Arguments:

depth The tree depth to plot for each tree in the forest.

root_label The label of the root node(s) in the plot.

plot Whether to create a plot or return the data used to generate the plot.

Returns: A data frame of parent-child relationships used to generate the igraph plot OR a ggplot2 object

Method to_vector(): Output all sequences held by the forest as a character vector

Usage:

RadixForest\$to_vector()

Returns: A character vector of all sequences contained in the forest.

Method size(): Output the size of the forest (i.e. how many sequences are contained)

Usage: RadixForest\$size()

Returns: The size of the forest

Method insert(): Insert new sequences into the forest

Usage:

RadixForest\$insert(sequences)

Arguments:

sequences A character vector of sequences to insert into the forest

Returns: A logical vector indicating whether the sequence was inserted (TRUE) or already existing in the forest (FALSE)

Method erase(): Erase sequences from the forest

Usage:

RadixForest\$erase(sequences)

Arguments:

sequences A character vector of sequences to erase from the forest

Returns: A logical vector indicating whether the sequence was erased (TRUE) or not found in the forest (FALSE)

Method find(): Find sequences in the forest

Usage: RadixForest\$find(query)

Arguments:

query A character vector of sequences to find in the forest

Returns: A logical vector indicating whether the sequence was found (TRUE) or not found in the forest (FALSE)

Method prefix_search(): Search for sequences in the forest that start with a specified prefix. E.g.: a query of "CAR" will find "CART", "CARBON", "CARROT", etc. but not "CATS".

Usage: RadixForest\$prefix_search(query) Arguments: query A character vector of sequences to search for in the forest Returns: A data frame of all matches with columns "query" and "target".

Method search(): Search for sequences in the forest that are with a specified distance metric to a specified query.

```
Usage:
RadixForest$search(
  query,
  max_distance = NULL,
  max_fraction = NULL,
  mode = "levenshtein",
  nthreads = 1,
  show_progress = FALSE
)
```

```
Arguments:
```

query A character vector of query sequences.

max_distance how far to search in units of absolute distance. Can be a single value or a vector. Mutually exclusive with max_fraction.

max_fraction how far to search in units of relative distance to each query sequence length. Can be a single value or a vector. Mutually exclusive with max_distance.

mode The distance metric to use. One of hamming (hm), global (gb) or anchored (an).

nthreads The number of threads to use for parallel computation.

show_progress Whether to show a progress bar.

Returns: The output is a data.frame of all matches with columns "query" and "target".

Method validate(): Validate the forest

Usage:

RadixForest\$validate()

Returns: A logical indicating whether the forest is valid (TRUE) or not (FALSE). This is mostly an internal function for debugging purposes and should always return TRUE.

```
forest <- RadixForest$new()
forest$insert(c("ACGT", "AAAA"))
forest$erase("AAA")
forest$search("ACG", max_distance = 1, mode = "levenshtein")
    # query target distance
    # 1 ACG ACGT 1
forest$search("ACG", max_distance = 1, mode = "hamming")
    # query target distance
    # <0 rows> (or 0-length row.names)
```

RadixTree

Description

Radix Tree (trie) class implementation

Details

The RadixTree class is a trie implementation. The primary usage is to be able to search of similar sequences based on a dynamic programming framework. This can be done using the *search* method which searches for similar sequences based on the Global, Anchored or Hamming distance metrics.

Three types of distance metrics are supported, based on the form of alignment performed. These are: Hamming, Global (Levenshtein) and Anchored.

An anchored alignment is a form of semi-global alignment, where the query sequence is "anchored" (global) to the beginning of both the query and target sequences, but is semi-global in that the end of the either the query sequence or target sequence (but not both) can be unaligned. This type of alignment is sometimes called an "extension" alignment in literature.

In contrast a global alignment must align the entire query and target sequences. When mismatch and indel costs are equal to 1, this is also known as the Levenshtein distance.

By default, if mode == "global" or "anchored", all mismatches and indels are given a cost of 1. However, you can define your own distance metric by setting the cost_matrix and gap parameters. The cost_matrix is a strictly positive square integer matrix and should include all characters in query and target as column- and rownames. To set the cost of a gap (insertion or deletion) you can include a row and column named "gap" in the cost_matrix *OR* set the gap_cost parameter (a single positive integer). Similarly, the affine gap alignment can be set by including a row and column named "gap_open" in the cost_matrix *OR* setting the gap_open_cost parameter (a single positive integer). If affine alignment is used, the cost of a gap is defined as: TOTAL_GAP_COST = gap_open_cost + (gap_cost * gap_length).

If mode == "hamming" all alignment parameters are ignored; mismatch is given a distance of 1 and gaps are not allowed.

Public fields

root_pointer Root of the RadixTree

char_counter_pointer Character count data for the purpose of validating input

Methods

Public methods:

- RadixTree\$new()
- RadixTree\$show()
- RadixTree\$to_string()
- RadixTree\$graph()

RadixTree

- RadixTree\$to_vector()
- RadixTree\$size()
- RadixTree\$insert()
- RadixTree\$erase()
- RadixTree\$find()
- RadixTree\$prefix_search()
- RadixTree\$search()
- RadixTree\$validate()

Method new(): Create a new RadixTree object

Usage: RadixTree\$new(sequences = NULL) Arguments:

sequences A character vector of sequences to insert into the tree

Method show(): Print the tree to screen

Usage: RadixTree\$show()

Method to_string(): Print the tree to a string

Usage: RadixTree\$to_string()

Returns: A string representation of the tree

Method graph(): Plot of the tree using igraph (needs to be installed separately)

Usage:

RadixTree\$graph(depth = -1, root_label = "root", plot = TRUE)

Arguments:

depth The tree depth to plot. If -1 (default), plot the entire tree.

root_label The label of the root node in the plot.

plot Whether to create a plot or return the data used to generate the plot.

Returns: A data frame of parent-child relationships used to generate the igraph plot OR a ggplot2 object

Method to_vector(): Output all sequences held by the tree as a character vector

Usage:

RadixTree\$to_vector()

Returns: A character vector of all sequences contained in the tree. Return order is not guaranteed.

Method size(): Output the size of the tree (i.e. how many sequences are contained)

Usage: RadixTree\$size() *Returns:* The size of the tree

Method insert(): Insert new sequences into the tree

Usage:

RadixTree\$insert(sequences)

Arguments:

sequences A character vector of sequences to insert into the tree

Returns: A logical vector indicating whether the sequence was inserted (TRUE) or already existing in the tree (FALSE)

Method erase(): Erase sequences from the tree

Usage:

RadixTree\$erase(sequences)

Arguments:

sequences A character vector of sequences to erase from the tree

Returns: A logical vector indicating whether the sequence was erased (TRUE) or not found in the tree (FALSE)

Method find(): Find sequences in the tree

Usage:

RadixTree\$find(query)

Arguments:

query A character vector of sequences to find in the tree

Returns: A logical vector indicating whether the sequence was found (TRUE) or not found in the tree (FALSE)

Method prefix_search(): Search for sequences in the tree that start with a specified prefix. E.g.: a query of "CAR" will find "CART", "CARBON", "CARROT", etc. but not "CATS".

Usage:

RadixTree\$prefix_search(query)

Arguments:

query A character vector of sequences to search for in the tree

Returns: A data frame of all matches with columns "query" and "target".

Method search(): Search for sequences in the tree that are with a specified distance metric to a specified query.

```
Usage:
RadixTree$search(
  query,
  max_distance = NULL,
  max_fraction = NULL,
  mode = "levenshtein",
  cost_matrix = NULL,
```

```
gap_cost = NULL,
gap_open_cost = NULL,
nthreads = 1,
show_progress = FALSE
```

Arguments:

)

query A character vector of query sequences.

- max_distance how far to search in units of absolute distance. Can be a single value or a vector. Mutually exclusive with max_fraction.
- max_fraction how far to search in units of relative distance to each query sequence length. Can be a single value or a vector. Mutually exclusive with max_distance.
- mode The distance metric to use. One of hamming (hm), global (gb) or anchored (an).
- cost_matrix A custom cost matrix for use with the "global" or "anchored" distance metrics. See details.
- gap_cost The cost of a gap for use with the "global" or "anchored" distance metrics. See details.

gap_open_cost The cost of a gap opening. See details.

nthreads The number of threads to use for parallel computation.

show_progress Whether to show a progress bar.

Returns: The output is a data.frame of all matches with columns "query" and "target". For anchored searches, the output also includes attributes "query_size" and "target_size" which are vectors containing the portion of the query and target sequences that are aligned.

Method validate(): Validate the tree

Usage:

RadixTree\$validate()

Returns: A logical indicating whether the tree is valid (TRUE) or not (FALSE). This is mostly an internal function for debugging purposes and should always return TRUE.

See Also

https://en.wikipedia.org/wiki/Radix_tree

```
tree <- RadixTree$new()
tree$insert(c("ACGT", "AAAA"))
tree$erase("AAAA")
tree$search("ACG", max_distance = 1, mode = "levenshtein")
# query target distance
# 1 ACG ACGT 1
tree$search("ACG", max_distance = 1, mode = "hamming")
# query target distance
# <0 rows> (or 0-length row.names)
```

split_search

Description

Search for similar sequences based on splitting sequences into left and right sides and searching for matches in each side using a bi-directional anchored alignment.

Usage

```
split_search(
  query,
  target,
  query_split,
  target_split,
  edge_trim = 0L,
  max_distance = 0L,
  ...
```

)

Arguments

query	A character vector of query sequences.
target	A character vector of target sequences.
query_split	index to split query sequence. Should be within (edge_trim, nchar(query)-edge_trim] or -1 to indicate no split.
target_split	index to split target sequence. Should be within (edge_trim, nchar(query)-edge_trim] or -1 to indicate no split.
edge_trim	number of bases to trim from each side of the sequence (default value: 0).
<pre>max_distance</pre>	how far to search in units of absolute distance. Can be a single value or a vector. Mutually exclusive with max_fraction.
	additional arguments passed to RadixTree\$search

Details

This function is useful for searching for similar sequences that may have variable windows of sequencing (e.g. different 5' and 3' primers) but contain the same core sequence or position. The two split parameters partition the query and target sequences into left and right sides, where left = $stri_sub(sequence, edge_trim+1, split)$ and right = $stri_sub(query, split+1, -edge_trim-1)$.

Value

data.frame with columns query, target, and distance.

split_search

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