

Package ‘immApex’

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Title Tools for Adaptive Immune Receptor Sequence-Based Machine and Deep Learning

Version 1.5.2

Description A set of tools to for machine and deep learning in R from amino acid and nucleotide sequences focusing on adaptive immune receptors. The package includes pre-processing of sequences, unifying gene nomenclature usage, encoding sequences, and combining models. This package will serve as the basis of future immune receptor sequence functions/packages/models compatible with the scRepertoire ecosystem.

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Description

A set of tools to for machine and deep learning in R from amino acid and nucleotide sequences focusing on adaptive immune receptors. The package includes pre-processing of sequences, unifying gene nomenclature usage, encoding sequences, and combining models. This package will serve as the basis of future immune receptor sequence functions/packages/models compatible with the scRepertoire ecosystem.

Author(s)

Maintainer: Nick Borcharding <ncborch@gmail.com>

See Also

Useful links:

- <https://github.com/BorchLab/immApex/>
- Report bugs at <https://github.com/BorchLab/immApex/issues>

ace_richness	<i>ACE Richness Estimator</i>
--------------	-------------------------------

Description

Calculates the Abundance-based Coverage Estimator (ACE) of species richness. This metric is particularly useful for datasets with a large number of rare species.

Usage

```
ace_richness(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Details

$$S_{ace} = S_{abund} + \frac{S_{rare}}{C_{ace}} + \frac{F_1}{C_{ace}} \gamma_{ace}^2$$

where the classification of rare and abundant species is based on a threshold of 10 individuals, *F*1 is the count of singletons, *S*rare is the number of rare species, and *C*ace is the sample coverage for rare species.

Value

A single numeric value representing the estimated total number of species. The estimate is constrained to be at least the number of observed species.

References

Chao, A., & Lee, S.-M. (1992). *Estimating the number of classes via sample coverage*. Journal of the American Statistical Association, 87(417), 210-217.

Examples

```
counts <- rpois(50, lambda=1.5)
ace_richness(counts)
```

adjacencyMatrix

Adjacency Matrix From Amino Acid or Nucleotide Sequences

Description

Calculate frequency of adjacency between residues along a set of biological sequences.

Usage

```
adjacencyMatrix(
  input.sequences,
  normalize = TRUE,
  sequence.dictionary = amino.acids,
  directed = FALSE
)
```

Arguments

input.sequences	Character vector of sequences (amino acid or nucleotide)
normalize	Return the values as a normalized frequency (TRUE) or raw counts (FALSE).
sequence.dictionary	The letters to use in the matrix (defaults to a standard 20 amino acids).
directed	Logical; if FALSE (default) the matrix is symmetrised.

Value

An adjacency matrix.

Examples

```
# new.sequences <- generateSequences(prefix.motif = "CAS",
#                                     suffix.motif = "YF",
#                                     number.of.sequences = 100,
#                                     min.length = 8,
#                                     max.length = 16)
# adj.matrix <- adjacencyMatrix(new.sequences,
#                                normalize = TRUE)
```

amino.acids	<i>Standard 20 amino acids</i>
-------------	--------------------------------

Description

Vector of one-letter codes for the 20 standard amino acids.

Usage

```
amino.acids
```

Format

An object of class character of length 20.

buildNetwork	<i>Build Edit Distance Network</i>
--------------	------------------------------------

Description

Build a sequence similarity network using various distance metrics and normalization options. Supports Levenshtein, Hamming, Damerau-Levenshtein, Needleman-Wunsch, and Smith-Waterman distances.

Usage

```
buildNetwork(  
  input.data = NULL,  
  input.sequences = NULL,  
  seq_col = NULL,  
  v_col = NULL,  
  j_col = NULL,  
  threshold = 2,  
  dist_type = "levenshtein",  
  dist_mat = NULL,  
  normalize = c("none", "length", "maxlen"),  
  gap_open = -10,  
  gap_extend = -1,  
  filter.v = FALSE,  
  filter.j = FALSE,  
  ids = NULL,  
  output = c("edges", "sparse"),  
  weight = c("dist", "binary")  
)
```

Arguments

<code>input.data</code>	'data.frame'/'tibble' with sequence & metadata (optional - omit if you supply 'sequences' directly).
<code>input.sequences</code>	Character vector of sequences **or** column name inside 'input.data'. Ignored when 'NULL' and 'seq_col' is non-'NULL'.
<code>seq_col, v_col, j_col</code>	Column names to use when 'input.data' is given. By default the function looks for common AIRR names ('junction_aa', 'cdr3', 'v_call', 'j_call').
<code>threshold</code>	≥ 1 for absolute distance **or** $0 < x \leq 1$ for relative. When using normalized distances ('normalize != "none"'), this typically should be a value between 0 and 1 (e.g., 0.9 for 10 percent dissimilarity).
<code>dist_type</code>	Character string specifying the distance metric to use: "levenshtein" - Standard edit distance (default, backward compatible) "hamming" - Hamming distance (requires equal-length sequences) "damerau" - Damerau-Levenshtein (allows transpositions) "nw" - Needleman-Wunsch global alignment score "sw" - Smith-Waterman local alignment score
<code>dist_mat</code>	Character string specifying which substitution matrix to use for alignment-based metrics ("nw", "sw"). Options include: "BLOSUM45" - BLOSUM45 matrix (distantly related) "BLOSUM50" - BLOSUM50 matrix "BLOSUM62" - BLOSUM62 matrix (default, good for proteins) "BLOSUM80" - BLOSUM80 matrix (closely related) "BLOSUM100" - BLOSUM100 matrix (very closely related) "PAM30" - PAM30 matrix (closely related sequences) "PAM40" - PAM40 matrix "PAM70" - PAM70 matrix "PAM120" - PAM120 matrix "PAM250" - PAM250 matrix (distantly related)
<code>normalize</code>	Character string specifying how to normalize distances: "none" - Raw distance values (default, backward compatible) "maxlen" - Normalize by $\max(\text{length}(\text{seq1}), \text{length}(\text{seq2}))$ "length" - Normalize by mean sequence length
<code>gap_open</code>	Gap opening penalty for alignment-based metrics (default: -10). Only used when 'metric' is "nw" or "sw".
<code>gap_extend</code>	Gap extension penalty for alignment-based metrics (default: -1). Only used when 'metric' is "nw" or "sw".
<code>filter.v</code>	Logical; require identical V when 'TRUE'.
<code>filter.j</code>	Logical; require identical J when 'TRUE'.
<code>ids</code>	Optional character labels; recycled from row-names if missing.
<code>output</code>	"edges" (default) or "sparse" - return an edge-list 'data.frame' **or** a symmetric 'Matrix::dgCMatrix' adjacency matrix.
<code>weight</code>	"dist" (store the edit distance) **or** "binary" (all edges get weight 1). Ignored when 'output = "edges"'.

Value

edge-list 'data.frame' ****or**** sparse adjacency 'dgCMatrix'

Examples

```
data(immapex_example.data)

# Levenshtein distance
edges <- buildNetwork(input.data = immapex_example.data[["AIRR"]],
                      seq_col   = "junction_aa",
                      threshold = 0.9,
                      filter.v  = TRUE)

# Using Hamming distance with normalization
edges <- buildNetwork(input.data = immapex_example.data[["AIRR"]],
                      seq_col   = "junction_aa",
                      threshold = 0.1,
                      dist_type = "hamming",
                      normalize = "maxlen",
                      filter.v  = TRUE)

# Using Needleman-Wunsch with BLOSUM62
edges <- buildNetwork(input.data = immapex_example.data[["AIRR"]],
                      seq_col   = "junction_aa",
                      threshold = 0.2,
                      dist_type = "nw",
                      normalize = "maxlen",
                      dist_mat  = "BLOSUM62",
                      filter.v  = TRUE)

# Using PAM30 for closely related sequences
edges <- buildNetwork(input.data = immapex_example.data[["AIRR"]],
                      seq_col   = "junction_aa",
                      threshold = 0.15,
                      dist_type = "nw",
                      normalize = "maxlen",
                      dist_mat  = "PAM30",
                      filter.v  = TRUE)

# Damerau-Levenshtein (allows transpositions)
edges <- buildNetwork(input.data = immapex_example.data[["AIRR"]],
                      seq_col   = "junction_aa",
                      threshold = 2,
                      dist_type = "damerau",
                      filter.v  = TRUE)
```

calculateEntropy

Positional Entropy / Diversity Biological Sequences

Description

Computes residue-wise diversity for a set of aligned (right-padded) CDR3 amino-acid sequences using ***any*** supported diversity estimator in ****immapex****. The following metrics are recognized:

***Shannon entropy:** `shannon_entropy` ***Inverse Simpson:** `inv_simpson` ***Gini–Simpson index:** `gini_simpson` ***Normalized entropy:** `norm_entropy` ***Pielou evenness:** `pielou_evenness` ***Hill numbers** (orders 0, 1, 2): `hill_q(0)`, `hill_q(1)`, `hill_q(2)`

You may also supply a *custom function* to `method`; it must take a numeric vector of clone counts and return a single numeric value.

Usage

```
calculateEntropy(
  input.sequences,
  max.length = NULL,
  method = c("shannon", "inv.simpson", "gini.simpson", "norm.entropy", "pielou", "hill0",
             "hill1", "hill2"),
  padding.symbol = "."
)
```

Arguments

`input.sequences` `'character()'`. Vector of CDR3 AA strings.

`max.length` `'integer(1)'`. Target length to align / pad to. **Default** = `'max(nchar(sequences))'`.

`method` Either the name of a built-in metric (`"shannon"`, `"inv.simpson"`, `"gini.simpson"`, `"norm.entropy"`, `"pielou"`, `"hill0"`, `"hill1"`, `"hill2"`) ***or*** a custom function as described above.

`padding.symbol` Symbol to use for padding at the end of sequences.

Value

Named `'numeric()'` vector of diversity scores, one value per position (Pos1 ... Pos*L*).

Examples

```
seqs <- c("CASSLGQDTQYF", "CASSIRSSYNEQFF", "CASSTGELFF")
calculateEntropy (seqs, method = "shannon")
```

calculateFrequency	<i>Relative Residue Frequencies at Every Position</i>
--------------------	---

Description

Quickly computes the per-position relative frequency of each symbol (amino-acid or nucleotide) in a set of biological sequences. Variable-length strings are padded to a common width so the calculation is entirely vectorized (one logical comparison + one `'colSums()'` per residue).

Usage

```
calculateFrequency(
  input.sequences,
  max.length = NULL,
  sequence.dictionary = amino.acids,
  padding.symbol = ".",
  summary.fun = c("proportion", "count", "percent"),
  tidy = FALSE
)
```

Arguments

<code>input.sequences</code>	Character vector of sequences (amino acid or nucleotide)
<code>max.length</code>	Integer. Pad/trim to this length. Defaults to <code>'max(nchar(sequences))'</code> .
<code>sequence.dictionary</code>	Vector of valid residue symbols that should be tracked (defaults to the 20 canonical amino acids; supply <code>'c("A","C","G","T","N")'</code> etc. for nucleotides).
<code>padding.symbol</code>	Single character used for right-padding. Must not be present in <code>'sequence.dictionary'</code> .
<code>summary.fun</code>	Character string choosing the summary statistic: <code>'"proportion"'</code> (default) – each cell sums to 1 over the table. <code>'"count"'</code> – raw counts. <code>'"percent"'</code> – $\text{proportion} \times 100$.
<code>tidy</code>	Logical; if <code>'TRUE'</code> a long-format <code>'data.frame'</code> is returned instead of a matrix (useful for plotting with <code>'ggplot2'</code>).

Value

Either

- A numeric matrix of dimension `'length(sequence.dictionary)' × 'max.length'`, whose columns sum to 1, **or**
- A `'data.frame'` with columns `'position'`, `'residue'`, `'frequency'` when `'tidy = TRUE'`.

Examples

```
# Amino Acid example
seqs <- c("CASSLGQGAETQYF", "CASSPGQGDYEYF", "CASSQETQYF")
rel.freq <- calculateFrequency(seqs)
head(rel.freq[, 1:5])

# Nucleotide example
dna <- c("ATGCC", "ATGAC", "ATGGC")
calculateFrequency(dna,
  sequence.dictionary = c("A","C","G","T"),
  padding.symbol = "-",
  tidy = TRUE)
```

calculateGeneUsage	<i>Quantification of Gene-Locus Usage</i>
--------------------	---

Description

Computes either the **counts**, **proportions** (default), or **percentages** of one locus *or* a locus pair that are already present as columns in 'input.data'. No external dependencies.

Usage

```
calculateGeneUsage(
  input.data,
  loci,
  levels = NULL,
  summary.fun = c("proportion", "count", "percent")
)
```

Arguments

input.data	A data.frame whose rows are sequences / clones and whose columns named in 'loci' contain gene identifiers.
loci	Character vector of length 1 or 2 giving the column names.
levels	Optional list of length 1 or 2 with the full set of factor levels to include. Missing levels are filled with zeros. If 'NULL' (default) only observed levels appear.
summary.fun	Character string choosing the summary statistic: * "proportion" (default) – each cell sums to 1 over the table. * "count" – raw counts. * "percent" – proportion $\times$ 100.

Value

Named numeric **vector** (single locus) or numeric **matrix** (paired loci). For "proportion" and "percent" results sum to 1 or 100.

Examples

```
df <- data.frame(V = c("TRBV7-2", "TRBV7-2", "TRBV5-1"),
                 J = c("TRBJ2-3", "TRBJ2-5", "TRBJ2-3"))
calculateGeneUsage(df, "V", summary = "count")
calculateGeneUsage(df, c("V", "J"), summary = "percent")
```

Description

Rapidly enumerates and quantifies **contiguous** (and, optionally, single-gap discontinuous) amino-acid motifs across a set of sequences.

Usage

```
calculateMotif(
  input.sequences,
  motif.lengths = 2:5,
  min.depth = 3,
  discontinuous = FALSE,
  discontinuous.symbol = ".",
  nthreads = 1
)
```

Arguments

<code>input.sequences</code>	Character vector of sequences (amino acid or nucleotide)
<code>motif.lengths</code>	Integer vector of motif sizes (≥ 1). Default: <code>2:5</code> .
<code>min.depth</code>	Minimum count a motif must reach to be retained in the output (≥ 1). Default: <code>3</code> .
<code>discontinuous</code>	Logical; include single-gap motifs as well? Default: <code>FALSE</code> .
<code>discontinuous.symbol</code>	Single character representing the gap when <code>discontinuous = TRUE</code> . Default: <code>"."</code> .
<code>nthreads</code>	Integer number of OpenMP threads to use. <code>1</code> forces serial execution. Default: <code>1</code> .

Details

For every input sequence the algorithm slides windows of length `k` (`motif.lengths`) and increments a motif counter (`unordered_map`). If `discontinuous = TRUE`, each window is additionally copied `k` times, substituting one position at a time with `discontinuous.symbol` (default `"."`), yielding gapped motif patterns such as `"C.S"`.

Value

A `data.frame` with two columns:

motif Motif string (contiguous or gapped).

frequency Integer occurrence count across all sequences.

Examples

```
seqs <- c("CASSLGQDTQYF", "CASSAGQDTQYF", "CASSLGEDTQYF")
calculateMotif(seqs, motif.lengths = 3, min.depth = 2)
```

calculateProperty

*Position-wise Amino-Acid Property Profiles***Description**

Computes a range of summary statistics for property values of one or more AA property scales at every residue position of a set of protein (or peptide) sequences. The function is entirely vectorized: it first calls [`calculateFrequency()`] to obtain a residue-by-position **frequency** matrix **F** (each column sums to 1) and then performs a single matrix product.

Usage

```
calculateProperty(
  input.sequences,
  property.set = "atchleyFactors",
  summary.fun = "mean",
  transform = "none",
  max.length = NULL,
  padding.symbol = ".",
  tidy = FALSE
)
```

Arguments

input.sequences	Character vector of amino-acid strings.
property.set	Character string (one of the supported names) Defaults to <code>"atchleyFactors"</code> , but includes: <code>"crucianiProperties"</code> , <code>"FASGAI"</code> , <code>"kideraFactors"</code> , <code>"MSWHIM"</code> , <code>"ProtFP"</code> , <code>"stScales"</code> , <code>"tScales"</code> , <code>"VHSE"</code> , <code>"zScales"</code>
summary.fun	Character string (<code>"mean"</code> , <code>"median"</code> , <code>"sum"</code> , <code>"min"</code> , <code>"max"</code>), or a function accepting a numeric vector and returning length-1 numeric. Defaults to <code>"mean"</code> .
transform	Character string controlling a post-summary transformation. One of <code>"none"</code> (default), <code>"sqrt"</code> , <code>"log1p"</code> , <code>"zscore"</code> (row-wise), or <code>"minmax"</code> (row-wise).
max.length	Integer. Pad/trim to this length (<code>max(nchar(sequences))</code> by default).
padding.symbol	Single character used for right-padding. Must not be one of the 20 canonical residues.
tidy	Logical; if <code>TRUE</code> , return a long-format <code>'data.frame'</code>

Value

A numeric matrix ($k \times L$) **or** a tidy data.frame with columns scale, position, value.

Examples

```
set.seed(1)
seqs <- c("CASSLGQGAETQYF", "CASSPGQGDYEQYF", "CASSQETQYF")
aa.Atchley <- calculateProperty(seqs, property.set = "atchleyFactors")
```

chao1_richness

*Chao1 Richness Estimator***Description**

Calculates the Chao1 non-parametric estimator of species richness.

Usage

```
chao1_richness(cnt)
```

Arguments

cnt Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.

Details

The bias-corrected formula is used:

$$S_{chao1} = S_{obs} + \frac{F_1(F_1 - 1)}{2(F_2 + 1)}$$

where *S*obs is the number of observed species, *F*1 is the count of singletons, and *F*2 is the count of doubletons.

If the conditions for the formula are not met (*F*1 <= 1 or *F*2 = 0), the function returns the observed richness (*S*obs).

Value

A single numeric value representing the estimated total number of species.

References

Chao, A. (1984). *Nonparametric estimation of the number of classes in a population*. Scandinavian Journal of Statistics, 11(4), 265-270.

Examples

```
# Sample with singletons and doubletons
counts <- c(rep(1, 10), rep(2, 5), 5, 8, 12)
chao1_richness(counts)

# Sample without doubletons returns observed richness
chao1_richness(c(rep(1, 5), 3, 4, 5))
```

d50_dom	<i>D50 Dominance Index</i>
---------	----------------------------

Description

A convenience wrapper for ‘dxx_dom(cnt, 50)’. Calculates the minimum number of top clones required to constitute 50

Usage

```
d50_dom(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Value

The smallest number of categories whose cumulative abundance is at least 50

Examples

```
d50_dom(c(100, 50, 20, 10, 5, rep(1, 5)))
```

dxx_dom	<i>Dxx Dominance Index</i>
---------	----------------------------

Description

Calculates the minimum number of top clones/sequences (ranked by abundance) that constitute a specified percentage of the total dataset. This function allows the user to designate the percentage.

Usage

```
dxx_dom(cnt, pct)
```

Arguments

cnt	Numeric vector of non-negative counts.
pct	A numeric value (0-100) for the target percentage.

Value

The smallest number of categories whose cumulative abundance is at least ‘pct’ percent of the total abundance.

See Also

```
[d50_dom()]
```

Examples

```
counts <- c(100, 50, 20, 10, 5, rep(1, 5))
dxx_dom(counts, 80)
```

formatGenes

*Ensure clean gene nomenclature using IMGT annotations***Description**

This function will format the genes into a clean nomenclature using the IMGT conventions.

Usage

```
formatGenes(
  input.data,
  region = "v",
  technology = NULL,
  species = "human",
  simplify.format = TRUE
)
```

Arguments

input.data	Data frame of sequencing data or scRepertoire outputs
region	Sequence gene loci to access - "v", "d", "j", or "c" or a combination using c("v", "d", "j")
technology	The sequencing technology employed - 'TenX' , 'Adaptive' , or 'AIRR'
species	One or two word designation of species. Currently supporting: "human", "mouse", "rat", "rabbit", "rhesus monkey", "sheep", "pig", "platypus", "alpaca", "dog", "chicken", and "ferret"
simplify.format	If applicable, remove the allelic designation (TRUE) or retain all information (FALSE)

Value

A data frame with the new columns of formatted genes added.

Examples

```
data(immapex_example.data)
formatGenes(immapex_example.data[["TenX"]],
  region = "v",
  technology = "TenX")
```

generateSequences	<i>Randomly Generate Amino Acid Sequences</i>
-------------------	---

Description

Use this to make synthetic amino acid sequences for purposes of testing code, training models, or providing noise.

Usage

```
generateSequences(
  prefix.motif = NULL,
  suffix.motif = NULL,
  number.of.sequences = 100,
  min.length = 1,
  max.length = 10,
  verbose = TRUE,
  sequence.dictionary = amino.acids
)
```

Arguments

prefix.motif	A defined amino acid/nucleotide sequence to add to the start of the generated sequences.
suffix.motif	A defined amino acid/nucleotide sequence to add to the end of the generated sequences.
number.of.sequences	The number of sequences to generate.
min.length	The minimum length of the final sequence. If this value is too short to fit the motifs, it will be automatically increased.
max.length	The maximum length of the final sequence. If it is less than the final 'min.length', it will also be adjusted.
verbose	Logical. If TRUE, prints messages when arguments like 'min.length' or 'max.length' are automatically adjusted.
sequence.dictionary	A character vector of the letters to use in random sequence generation.

Value

A character vector of generated sequences.

Examples

```
generateSequences(prefix.motif = "CAS",
  suffix.motif = "YF",
  number.of.sequences = 100,
  min.length = 8,
  max.length = 16)
```

Description

Use this to access the ImMunoGeneTics (IMGT) sequences for a specific species and gene loci. More information on IMGT can be found at imgt.org.

Usage

```
getIMGT(  
  species = "human",  
  chain = "TRB",  
  sequence.type = "aa",  
  frame = "inframe",  
  region = "v",  
  max.retries = 3,  
  verbose = TRUE  
)
```

Arguments

species	One or two-word common designation of species.
chain	Sequence chain to access, e.g., TRB or IGH .
sequence.type	Type of sequence - aa (amino acid) or nt (nucleotide).
frame	Designation for all , inframe , or inframe+gap .
region	Gene loci to access.
max.retries	Number of attempts to fetch data in case of failure.
verbose	Print messages corresponding to the processing step.

Value

A list of allele sequences.

Examples

```
## Not run:  
TRBV_aa <- getIMGT(species = "human",  
  chain = "TRB",  
  frame = "inframe",  
  region = "v",  
  sequence.type = "aa",  
  max.retries = 3)  
  
## End(Not run)
```

getIR

Extract Immune Receptor Sequences

Description

Use this to extract immune receptor sequences from a Single-Cell Object or the output of [combineTCR](#) and [combineBCR](#).

Usage

```
getIR(
  input.data,
  chains,
  sequence.type = c("aa", "nt"),
  group.by = NULL,
  as.list = FALSE
)
```

Arguments

input.data	Single-cell object or the output of combineTCR and combineBCR from scReptoire
chains	Immune Receptor chain to use - TRA , TRB , IGH , or IGL
sequence.type	Extract amino acid (aa) or nucleotide (nt) sequences
group.by	Optional metadata column (e.g., "sample.id") to group and return results as a named list by that variable.
as.list	Logical; if TRUE, returns a list split by chain. If group.by is also provided, returns a nested list Default is FALSE.

Value

A data frame, list of data frames, or nested list of immune receptor sequences depending on as.list and group.by. Each entry includes CDR3 sequence, V(D)J gene segments, and associated barcodes.

get_substitution_matrix

Get substitution matrix from package data or custom input

Description

Get substitution matrix from package data or custom input

Usage

```
get_substitution_matrix(matrix_name)
```

Arguments

matrix_name Character string or numeric matrix

Value

Numeric matrix with amino acid row/column names

gini_coef	<i>Gini Coefficient of Abundance Inequality</i>
-----------	---

Description

Calculates the Gini coefficient, a measure of inequality, for a vector of clone/sequence counts. It ranges from 0 (perfect equality) to nearly 1 (maximal inequality).

Usage

```
gini_coef(cnt)
```

Arguments

cnt Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.

Details

$$G = \frac{\sum_{i=1}^S (2i - S - 1)n_i}{S \sum_{i=1}^S n_i}$$

where *n_i* are the counts of each of the *S* categories, sorted in non-decreasing order.

Value

A numeric value in [0, 1]. Returns '0' if there is only one category.

See Also

[gini_simpson()]

Examples

```
# High inequality
gini_coef(c(100, 1, 1, 1))
# Perfect equality
gini_coef(c(10, 10, 10, 10))
```

gini_simpson	<i>Gini–Simpson Diversity</i>
--------------	-------------------------------

Description

Computes the complement of Simpson’s index (also called the Gini–Simpson index or probability of interspecific encounter):

Usage

```
gini_simpson(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Details

$$1 - \lambda = 1 - \sum_i p_i^2$$

Value

Value in the interval [0, 1]. Higher numbers indicate greater heterogeneity.

Examples

```
gini_simpson(c(10, 5, 5))
```

hill_q	<i>Hill-Number Generator</i>
--------	------------------------------

Description

Returns a *function* that computes the Hill diversity of order *q* (also called the “effective number of species”):

Usage

```
hill_q(q)
```

Arguments

q	Numeric order of diversity. Common values: <i>0</i> (richness), <i>1</i> ($\exp(H)$), <i>2</i> (inverse Simpson).
---	---

Details

$${}^qD = \left(\sum_i p_i^q \right)^{1/(1-q)}, \quad q \neq 1$$

For $q = 1$ the formula is undefined; the limit is

$${}^1D = e^{H'}$$

.

Value

A **closure**: `hill_q(q)` returns a function that takes a vector of counts and yields the corresponding qD . The returned function is vectorised over its input.

References

Hill, M. O. (1973) *Diversity and Evenness: A Unifying Notation and its Consequences*. *Ecology* **54** (2), 427–432.

Examples

```
hill1 <- hill_q(1) # q = 1
hill1(c(5, 1, 1, 1))

hill2 <- hill_q(2) # q = 2, inverse-Simpson
hill2(c(5, 1, 1, 1))
```

immapex_blosum.pam.matrices

List of amino acid substitution matrices

Description

A list of amino acid substitution matrices, using the Point Accepted Matrix (PAM) and BLOck Substitution Matrix (BLOSUM) approaches. A discussion and comparison of these matrices are available at [PMID: 21356840](#).

- BLOSUM45
- BLOSUM50
- BLOSUM62
- BLOSUM80
- BLOSUM100
- PAM30
- PAM40
- PAM70
- PAM120
- PAM250

Usage

```
data("immapex_blosum.pam.matrices")
```

Value

List of 10 substitution matrices

```
immapex_example.data
```

Example contig data for Apex

Description

Contains a collection of bulk or paired TCR sequences in the respective formats in the form of a list from the following sources:

- TenX: 10k_Human_DTC_Melanoma_5p_nextgem_Multiplex from [10x Website](#).
- AIRR: Human_colon_16S8157851 from [PMID: 37055623](#).
- Adaptive: Adaptive_2283_D0 from [PMID: 36220826](#).

More information on the data formats are available: [AIRR](#), [Adaptive](#), and [TenX](#).

Usage

```
data("immapex_example.data")
```

Value

List of 3 example data sets for 10x, AIRR and Adaptive contigs.

```
immapex_gene.list
```

A list of IMGT gene names by genes, loci, and species

Description

A list of regularized gene nomenclature to use for converting for data for uniformity. Data is organized by gene region, loci and species. Not all species are represented in the data and pseudogenes have not been removed.

Usage

```
data("immapex_gene.list")
```

Value

List of gene nomenclature by region, loci, and species.

inferCDR

*Infer CDR-loop segments from V-gene calls***Description**

Use this isolate sequences from the CDR loop using the V gene annotation. When there are multiple V gene matches for a single gene, the first allelic sequence is used.

Usage

```
inferCDR(
  input.data,
  reference,
  chain = "TRB",
  technology = c("TenX", "AIRR", "Adaptive", "Omniscope"),
  sequence.type = c("aa", "nt"),
  sequences = c("CDR1", "CDR2"),
  verbose = TRUE
)
```

Arguments

input.data	Data frame output of formatGenes
reference	IMGT reference sequences from getIMGT
chain	Sequence chain to access, like TRB or IGH
technology	The sequencing technology employed - TenX , Adaptive , or AIRR
sequence.type	Type of sequence - aa for amino acid or nt for nucleotide
sequences	The specific regions of the CDR loop to get from the data, such as CDR1 .
verbose	Logical. If 'TRUE' (default), prints a progress message.

Value

A data frame with the new columns of CDR sequences added.

Examples

```
## Not run:
# Getting the Sequence Reference
data(immapex_example.data)
TRBV_aa <- getIMGT(species = "human",
  chain = "TRB",
  frame = "inframe",
  region = "v",
  sequence.type = "aa")

# Ensuring sequences are formatted to IMGT
TenX_formatted <- formatGenes(immapex_example.data[["TenX"]],
  region = "v",
  technology = "TenX")

# Inferring CDR loop elements
```

```
TenX_formatted <- inferCDR(TenX_formatted,
  chain = "TRB",
  reference = TRBV_aa,
  technology = "TenX",
  sequence.type = "aa",
  sequences = c("CDR1", "CDR2"))

## End(Not run)
```

inv_simpson	<i>Inverse Simpson Diversity</i>
-------------	----------------------------------

Description

Computes the inverse of Simpson's concentration index, sometimes written as $1/D$. This metric emphasizes dominant categories.

Usage

```
inv_simpson(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Details

$$1/D = \frac{1}{\sum_i p_i^2}$$

Value

Numeric value ≥ 1 . Equals 1 when all observations belong to a single category.

Examples

```
inv_simpson(c(10, 5, 1))
```

make_identity_matrix	<i>Create a simple identity substitution matrix</i>
----------------------	---

Description

Create a simple identity substitution matrix

Usage

```
make_identity_matrix()
```

mutateSequences	<i>Randomly Mutate Sequences of Amino Acids</i>
-----------------	---

Description

Use this to mutate or mask sequences for purposes of testing code, training models, or noise.

Usage

```
mutateSequences(  
  input.sequences,  
  number.of.sequences = 1,  
  mutation.rate = 0.01,  
  position.start = NULL,  
  position.end = NULL,  
  sequence.dictionary = amino.acids  
)
```

Arguments

input.sequences	The amino acid or nucleotide sequences to use
number.of.sequences	The number of mutated sequences to return
mutation.rate	The rate of mutations to introduce into sequences
position.start	The starting position to mutate along the sequence Default = NULL will start the random mutations at position 1
position.end	The ending position to mutate along the sequence Default = NULL will end the random mutations at the last position
sequence.dictionary	The letters to use in sequence mutation (default are all amino acids)

Value

A vector of mutated sequences

Examples

```
sequences <- generateSequences(prefix.motif = "CAS",  
                               suffix.motif = "YF",  
                               number.of.sequences = 100,  
                               min.length = 8,  
                               max.length = 16)  
  
mutated_sequences <- mutateSequences(sequences,  
                                     number.of.sequences = 1,  
                                     position.start = 3,  
                                     position.end = 8)
```

norm_entropy	<i>Normalised Shannon Entropy</i>
--------------	-----------------------------------

Description

Shannon entropy scaled to the interval [0, 1] by its maximum possible value given *S* observed categories:

Usage

```
norm_entropy(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Details

$$H^* = \frac{H'}{\ln S}$$

(also known as “Shannon evenness”).

Value

Numeric value in [0, 1]; ‘0’ when all observations are in a single category.

Examples

```
norm_entropy(c(40, 10, 10, 10))
```

pielou_evenness	<i>Pielou’s Evenness</i>
-----------------	--------------------------

Description

Convenience wrapper for normalized Shannon entropy (*E* = *H* / ln *S*).

Usage

```
pielou_evenness(cnt)
```

Arguments

cnt	Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.
-----	--

Value

Numeric evenness measure in [0, 1].

Examples

```
pielou_evenness(c(3, 3, 3))
```

positionalEncoder	<i>Generate Sinusoidal Positional Encodings</i>
-------------------	---

Description

Creates a matrix of sinusoidal positional encodings as described in the "Attention Is All You Need" paper. This provides a way to inject information about the relative or absolute position of tokens in a sequence.

Usage

```
positionalEncoder(
  max.length = NULL,
  d.model = NULL,
  input.sequences = NULL,
  base = 10000,
  position.offset = 1L
)
```

Arguments

max.length	The maximum sequence length (number of positions) to encode. This is the primary way to specify the output size.
d.model	The dimensionality of the embedding. Must be an even number.
input.sequences	Optional. A character vector of sequences. If provided, 'max.length' is automatically determined from the longest sequence, unless 'max.length' is also explicitly set to a larger value.
base	The base for the geometric progression of frequencies. The default is 10000, as used in the original paper.
position.offset	An integer offset for position numbering. Defaults to 1 (1-based indexing common in R). Set to 0 for 0-based indexing.

Value

A matrix of shape 'max.length' x 'd.model' containing the positional encodings.

Details

The implementation uses the standard formulas: $PE(pos, 2i) = \sin(pos / base^{(2i / d.model)})$, $PE(pos, 2i+1) = \cos(pos / base^{(2i / d.model)})$ where 'pos' is the position, 'i' is the dimension pair, 'd.model' is the embedding dimension, and 'base' is a user-definable base, typically 10000.

Examples

```
pos_encoding <- positionalEncoder(max.length = 50,
                                  d.model = 64)

my_sequences <- c("SEQUENCE", "ANOTHERSEQ")
pos_enc_auto <- positionalEncoder(input.sequences = my_sequences,
                                  d.model = 32)
```

probabilityMatrix	<i>Position Probability Matrix for Amino Acid or Nucleotide Sequences</i>
-------------------	---

Description

Generates a position-probability (PPM) or position-weight (PWM) matrix from a set of biological sequences.

Usage

```
probabilityMatrix(
  input.sequences,
  max.length = NULL,
  convert.PWM = FALSE,
  background.frequencies = NULL,
  sequence.dictionary = amino.acids,
  pseudocount = 1,
  padding.symbol = "."
)
```

Arguments

input.sequences	Character vector of sequences.
max.length	Integer; sequences will be right-padded to this length. If NULL (default), pads to the length of the longest sequence in the input.
convert.PWM	Logical; if TRUE, converts the matrix into a PWM.
background.frequencies	Named vector of background frequencies for PWM calculation. If NULL, a uniform distribution is assumed. Names must correspond to characters in 'sequence.dictionary'.
sequence.dictionary	Character vector of residues to include in the matrix.
pseudocount	A small number added to raw counts for PWM calculation to avoid zero probabilities. Defaults to 1.
padding.symbol	Single character for right-padding. Must not be in 'sequence.dictionary'.

Value

A matrix with position-specific probabilities (PPM) or weights (PWM).

Examples

```
new.sequences <- generateSequences(prefix.motif = "CAS",
                                   suffix.motif = "YF",
                                   number.of.sequences = 100,
                                   min.length = 8,
                                   max.length = 16)

PPM.matrix <- probabilityMatrix(new.sequences)
```

scaleMatrix

Fast Matrix Scaling or Transformation

Description

Applies a chosen transformation to every row *or* column of a numeric matrix without altering its dimensions. Designed for lightweight pre-processing pipelines ahead of machine-learning models.

Usage

```
scaleMatrix(
  x,
  method = c("minmax", "z", "robust_z", "unit_var", "l2", "l1", "sqrt", "log1p", "log2",
             "log10", "arcsinh", "none"),
  margin = 2,
  range = c(0, 1),
  offset = 1e-08,
  cofactor = 5,
  na.rm = TRUE
)
```

Arguments

x	Numeric matrix (coerced with <code>as.matrix()</code>).
method	Character scalar. One of: • "minmax" – rescale linearly to [range]. • "z" – mean 0 / sd 1 (per margin). • "robust_z" – median 0 / MAD 1 (outlier-resistant). • "unit_var" – divide by sd (keep mean shifts). • "l2", "l1" – divide by Euclidean / L1 norm. • "sqrt" – element-wise square-root. • "log1p" – element-wise $\log_{10}(x + \text{offset})$. • "log2", "log10" – logs with small offset. • "arcsinh" – $\text{asinh}(x / \text{cofactor})$ (Flow/CyTOF). • "none" – return unchanged.
margin	1 = operate row-wise, 2 = column-wise (default 2).
range	Numeric length-2 vector for method = "minmax".
offset	Non-negative scalar added before logs / sqrt (<i>ignored</i> otherwise). Default 1e-8.
cofactor	Numeric > 0 for method = "arcsinh" (default 5).
na.rm	Logical; drop NAs when computing summaries.

Value

Matrix of identical dimension (dimnames preserved).

Examples

```
m <- matrix(rnorm(20), 4, 5,
            dimnames = list(paste0("g", 1:4), paste0("s", 1:5)))
scaleMatrix(m, "minmax")
scaleMatrix(m, "robust_z", margin = 1)
scaleMatrix(m, "l2")
scaleMatrix(abs(m), "arcsinh", cofactor = 150)
```

sequenceDecoder

*Decode Amino Acid or Nucleotide Sequences***Description**

Transforms one-hot or property-encoded sequences back into their original character representation. This function serves as the inverse to ‘sequenceEncoder’.

Usage

```
sequenceDecoder(
  encoded.object,
  mode = c("onehot", "property"),
  property.set = NULL,
  property.matrix = NULL,
  call.threshold = 0.5,
  sequence.dictionary = amino.acids,
  padding.symbol = ".",
  remove.padding = TRUE
)
```

Arguments

- | | |
|-----------------|--|
| encoded.object | A ‘list’ object produced by ‘sequenceEncoder’, or a numeric ‘matrix’ (flattened 2D) or ‘array’ (3D cube) from it. |
| mode | The encoding mode used for decoding: “onehot” or “property”. This is typically inferred if ‘encoded.object’ is a list from ‘sequenceEncoder’. |
| property.set | For ‘mode = “property”’, a character vector of property names (e.g., “atchley-Factors”) that were used for the original encoding. See ‘?sequenceEncoder’. This is ignored if ‘property.matrix’ is supplied. |
| property.matrix | For ‘mode = “property”’, the exact numeric matrix (with dimensions ‘20 x P’) that was used for encoding. This overrides ‘property.set’. |
| call.threshold | A numeric confidence threshold for making a call. - In “onehot” mode, this is the minimum required value in the vector (e.g., ‘0.9’). - In “property” mode, this is the maximum allowable Euclidean distance. Positions with scores not meeting the threshold are assigned the ‘padding.symbol’. |

sequence.dictionary A character vector of the alphabet (e.g., amino acids). Must match the one used during encoding.

padding.symbol The single character used to represent padding or low-confidence positions.

remove.padding Logical. If 'TRUE', trailing padding symbols are removed from the end of the decoded sequences.

Value

A character vector of the decoded sequences.

Examples

```
# Example sequences
aa.sequences <- c("CAR", "YMD", "ACAC")

# Encode the sequences
encoded.onehot <- sequenceEncoder(aa.sequences,
                                  mode = "onehot")
encoded.prop <- sequenceEncoder(aa.sequences,
                                mode = "property",
                                property.set = "atchleyFactors")

# Decode the sequences
# 1. Decode from the full list object
decoded.1 <- sequenceDecoder(encoded.onehot,
                              mode = "onehot")

# 2. Decode from just the 3D cube array
decoded.2 <- sequenceDecoder(encoded.prop$cube,
                              mode = "property",
                              property.set = "atchleyFactors")
```

sequenceEncoder

Universal Amino-acid Sequence Encoder

Description

'sequenceEncoder()' is a high-level function that converts a character vector of amino-acid sequences into one of three representations: 1. **one-hot**: A binary representation for each amino acid position. 2. **property-based**: A numerical representation based on amino acid properties (e.g., atchleyFactors, kideraFactors, etc). 3. **geometric**: A fixed-length 20-dimensional vector for each sequence, derived from a substitution matrix and geometric rotation.

Usage

```
sequenceEncoder(
  input.sequences,
  mode = c("onehot", "property", "geometric"),
  property.set = NULL,
  property.matrix = NULL,
```

```

    method = "BLOSUM62",
    theta = pi/3,
    sequence.dictionary = amino.acids,
    padding.symbol = ".",
    summary.fun = "",
    max.length = NULL,
    nthreads = parallel::detectCores(),
    verbose = TRUE,
    ...
)

onehotEncoder(..., mode = "onehot")

propertyEncoder(..., mode = "property")

geometricEncoder(..., mode = "geometric")

```

Arguments

<code>input.sequences</code>	<code>'character'</code> vector. Sequences (uppercase single-letter code).
<code>mode</code>	Either <code>"onehot"</code> , <code>"property"</code> , or <code>"geometric"</code> .
<code>property.set</code>	Character string (one of the supported names) Defaults to <code>"atchleyFactors"</code> , but includes: <code>"crucianiProperties"</code> , <code>"FASGAI"</code> , <code>"kideraFactors"</code> , <code>"MSWHIM"</code> , <code>"ProtFP"</code> , <code>"stScales"</code> , <code>"tScales"</code> , <code>"VHSE"</code> , <code>"zScales"</code> Ignored if <code>'property.matrix'</code> is supplied.
<code>property.matrix</code>	*Optional numeric matrix ($20 \times P$)*. Overrides <code>'property.set'</code> in <code>"property"</code> mode.
<code>method</code>	*(For geometric mode)* Character key for a built-in substitution matrix (e.g., <code>"BLOSUM62"</code>), or a 20x20 numeric matrix itself.
<code>theta</code>	*(For geometric mode)* Rotation angle in radians (default <code>'pi/3'</code>).
<code>sequence.dictionary</code>	Character vector of the alphabet (default = 20 standard amino acids).
<code>padding.symbol</code>	Single character for right-padding (non-geometric modes).
<code>summary.fun</code>	For property mode only: <code>"mean"</code> or <code>""</code> (none).
<code>max.length</code>	Integer for truncation/padding. If <code>'NULL'</code> (default), the longest sequence sets the maximum. Not used in geometric mode.
<code>nthreads</code>	Number of threads for C++ backend. Not used in geometric mode.
<code>verbose</code>	Logical. If <code>'TRUE'</code> (default), prints a progress message.
<code>...</code>	Additional arguments passed to <code>'sequenceEncoder()'</code> when using wrapper functions (<code>'onehotEncoder'</code> , <code>'propertyEncoder'</code> , <code>'geometricEncoder'</code>).

Details

The function acts as a wrapper for either the C++ backend (for one-hot and property modes) or the R-based geometric transformation.

Value

A named 'list' containing the encoded data and metadata.

'cube' 3D Numeric array. 'NULL' in geometric mode.

'flattened' 2D Numeric matrix. 'NULL' in geometric mode.

'summary' 2D Numeric matrix containing sequence-level representations. This is the primary output for geometric mode.

... Other metadata related to the encoding process.

Property Mode

If you supply 'property.matrix' directly, it **must** be a numeric matrix whose **rows** correspond to the 20 canonical amino acids in the order of 'sequence.dictionary' and whose columns are the property scales.

Geometric Mode

This mode projects sequences into a 20D space. It calculates the average vector for each sequence using a substitution matrix (e.g., "BLOSUM62") and then applies a planar rotation to the resulting vector.

Examples

```
aa <- c("CARDRST", "YYYGMD", "ACACACAC")

# One-hot encoding
enc_onehot <- sequenceEncoder(aa,
                              mode = "onehot")

# Property-based encoding
enc_prop <- sequenceEncoder(aa,
                            mode = "property",
                            property.set = "atchleyFactors")

# Geometric encoding
enc_geo <- sequenceEncoder(aa,
                           mode = "geometric",
                           method = "BLOSUM62")
```

shannon_entropy

Shannon Diversity Index (Entropy)

Description

Calculates Shannon's information entropy (often denoted H^*) for a set of clone or sequence counts.

Usage

```
shannon_entropy(cnt)
```

Arguments

cnt Numeric vector of non-negative counts (one entry per clone/ residue/OTU). Zero counts are ignored.

Details

$$H' = - \sum_{i=1}^S p_i \ln p_i$$

where $p_i = n_i / N$ are the relative frequencies (proportions) of each of the S distinct categories.

Value

A single numeric value (≥ 0). When ‘cnt’ contains exactly one positive entry the function returns ‘0’.

See Also

[norm_entropy()], [inv_simpson()]

Examples

```
counts <- c(A = 12, B = 4, C = 4)
shannon_entropy(counts)
```

summaryMatrix	<i>Fast Matrix Summaries</i>
---------------	------------------------------

Description

Computes a comprehensive panel of univariate statistics for every **row** or **column** of a numeric matrix. It is designed for lightweight feature-engineering pipelines where many summaries are required up-front (e.g. before modeling).

Usage

```
summaryMatrix(x, margin = 2, stats = "all", na.rm = TRUE)
```

Arguments

x Numeric matrix (will be coerced with `as.matrix()`).

margin Integer. 1 = operate row-wise; 2 = column-wise (default 2).

stats Character vector naming the statistics to return. Any combination of the following (case-insensitive):

- "min"
- "max"
- "mean"
- "median"

- "sd"
- "var"
- "mad"
- "sum",
- "iqr"
- "n"
- "na"
- "mode"
- "all"

na.rm Logical; ignore NAs when calculating statistics default TRUE).

Value

A numeric matrix with one **row** per object that was summarised (rows of the input when `margin = 1`, otherwise columns) and one **column** per requested statistic. Row-names (if present) are preserved; column names are the statistic labels.

Examples

```
m <- matrix(rnorm(20), 4, 5,
            dimnames = list(paste0("g", 1:4), paste0("s", 1:5)))

## Column-wise summaries (default)
head(summaryMatrix(m))

## Row-wise summaries
head(summaryMatrix(m, margin = 1))
```

tokenizeSequences	<i>Generate Tokenized Sequences from Amino Acid String</i>
-------------------	--

Description

Use this to transform amino acid sequences into tokens in preparing for deep learning models.

Usage

```
tokenizeSequences(
  input.sequences,
  add.startstop = TRUE,
  start.token = "!",
  stop.token = "^",
  max.length = NULL,
  convert.to.matrix = TRUE,
  padding.symbol = NULL,
  verbose = TRUE
)
```

Arguments

<code>input.sequences</code>	The amino acid or nucleotide sequences to use
<code>add.startstop</code>	Add start and stop tokens to the sequence
<code>start.token</code>	The character to use for the start token
<code>stop.token</code>	The character to use for the stop token
<code>max.length</code>	Additional length to pad, NULL will pad sequences to the max length of <code>input.sequences</code>
<code>convert.to.matrix</code>	Return a matrix (TRUE) or a vector (FALSE)
<code>padding.symbol</code>	Single character used for right-padding.
<code>verbose</code>	Print messages corresponding to the processing step

Value

Integer matrix (rows = sequences, cols = positions) or list of vectors.

Examples

```
new.sequences <- generateSequences(prefix.motif = "CAS",
                                   suffix.motif = "YF",
                                   number.of.sequences = 100,
                                   min.length = 8,
                                   max.length = 16)

sequence.matrix <- tokenizeSequences(new.sequences,
                                     add.startstop = TRUE,
                                     start.token = "!",
                                     stop.token = "^",
                                     convert.to.matrix = TRUE)
```

`variationalSequences` *Generate Similar Sequences using Variational Autoencoder (Defunct)*

Description

This function is defunct and no longer available.

Usage

```
variationalSequences(...)
```

Details

This function previously generated synthetic sequences using a variational autoencoder (VAE). It has been removed for maintenance and clarity.

Value

No return value, called for side effects only.

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