

Package: immApex (via r-universe)

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

Version 1.6.0

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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Encoding UTF-8

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|--------------|-------------------------------|
| 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

| | |
|----------------------------------|---|
| <code>input.sequences</code> | Character vector of sequences (amino acid or nucleotide) |
| <code>normalize</code> | Return the values as a normalized frequency (TRUE) or raw counts (FALSE). |
| <code>sequence.dictionary</code> | The letters to use in the matrix (defaults to a standard 20 amino acids). |
| <code>directed</code> | 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', 'sequence', 'seq'). |
| <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 0.0 and 1.0 (e.g., 0.1 for 10 percent dissimilarity). |
| <code>dist_type</code> | Character string specifying the distance metric to use: <ul style="list-style-type: none"> "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: <ul style="list-style-type: none"> "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: <ul style="list-style-type: none"> "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. |

output "edges" (default) or "sparse" - return an edge-list 'data.frame' **or** a symmetric 'Matrix::dgCMatrix' adjacency matrix.

weight "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' of distances

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 *Relative Residue Frequencies at Every Position*

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

`input.sequences` Character vector of sequences (amino acid or nucleotide)

`max.length` Integer. Pad/trim to this length. Defaults to `'max(nchar(sequences))'`.

`sequence.dictionary` Vector of valid residue symbols that should be tracked (defaults to the 20 canonical amino acids; supply `'c("A","C","G","T","N")'` etc. for nucleotides).

`padding.symbol` Single character used for right-padding. **Must not** be present in `'sequence.dictionary'`.

`summary.fun` Character string choosing the summary statistic: * `"proportion"` (default) – each cell sums to 1 over the table. * `"count"` – raw counts. * `"percent"` – proportion × 100.

`tidy` Logical; if `'TRUE'` a long-format `'data.frame'` is returned instead of a matrix (useful for plotting with `*ggplot2*`).

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", "CASSPGQGDYEQYF", "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 *Quantification of Gene-Locus Usage*

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 × 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")
```

calculateMotif *Motif Enumeration and Counting*

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

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

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 "atchleyFactors", but includes: "crucianiProperties", "FASGAI", "kideraFactors", "MSWHIM", "ProtFP", "stScales", "tScales", "VHSE", "zScales" |
| summary.fun | Character string ("mean", "median", "sum", "min", "max"), or a function accepting a numeric vector and returning length-1 numeric. Defaults to "mean". |
| transform | Character string controlling a post-summary transformation. One of "none" (default), "sqrt", "log1p", "zscore" (row-wise), or "minmax" (row-wise). |

max.length Integer. Pad/trim to this length ('max(nchar(sequences))' by default).

padding.symbol Single character used for right-padding. Must not be one of the 20 canonical residues.

tidy Logical; if 'TRUE', return a long-format 'data.frame'

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 | <i>Chao1 Richness Estimator</i> |
|----------------|---------------------------------|

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 ($F_1 \leq 1$ 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

D50 Dominance Index

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 | <i>Ensure clean gene nomenclature using IMGT annotations</i> |
|-------------|--|

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 *Randomly Generate Amino Acid Sequences*

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)
```

getIMGT

Get IMGT Sequences for Specific Loci

Description

Use this to access the ImMunoGeneTics (IMGT) sequences for a specific species and gene loci via the `immReferent` package, which provides automatic local caching. More information on IMGT can be found at imgt.org.

Usage

```
getIMGT(
  species = "human",
  chain = "TRB",
  sequence.type = "aa",
  region = "v",
  refresh = FALSE
)
```

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). |
| region | Gene loci to access - v , d , j , or c . |
| refresh | Logical. If TRUE, forces a re-download of the data even if cached locally. Default is FALSE. |

Value

A list containing sequences (a named list of allele sequences) and misc (metadata including species, chain, sequence.type, and region).

Examples

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

## 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 <code>combineTCR</code> and <code>combineBCR</code> from <code>scReper-</code> <code>toire</code> |
| 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 bar-codes.

| | |
|-----------|---|
| 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 *Hill-Number Generator*

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: *0* (richness), *1* ($\exp(H)$), *2* (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 | <i>A list of IMGT gene names by genes, loci, and species</i> |
|-------------------|--|

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 | <i>Infer CDR-loop segments from V-gene calls</i> |
|----------|--|

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",
                  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

Inverse Simpson Diversity

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))
```

mutateSequences *Randomly Mutate Sequences of Amino Acids*

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

| | |
|------------------------------|---|
| <code>max.length</code> | The maximum sequence length (number of positions) to encode. This is the primary way to specify the output size. |
| <code>d.model</code> | The dimensionality of the embedding. Must be an even number. |
| <code>input.sequences</code> | 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. |
| <code>base</code> | The base for the geometric progression of frequencies. The default is 10000, as used in the original paper. |
| <code>position.offset</code> | 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

| | |
|-------------------------------------|---|
| <code>input.sequences</code> | Character vector of sequences. |
| <code>max.length</code> | Integer; sequences will be right-padded to this length. If NULL (default), pads to the length of the longest sequence in the input. |
| <code>convert.PWM</code> | Logical; if TRUE, converts the matrix into a PWM. |
| <code>background.frequencies</code> | Named vector of background frequencies for PWM calculation. If NULL, a uniform distribution is assumed. Names must correspond to characters in ‘sequence.dictionary’. |
| <code>sequence.dictionary</code> | Character vector of residues to include in the matrix. |
| <code>pseudocount</code> | A small number added to raw counts for PWM calculation to avoid zero probabilities. Defaults to 1. |
| <code>padding.symbol</code> | 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: <ul style="list-style-type: none"> • "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 $\log_{1p}(x + \text{offset})$. • "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'.

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

| | |
|-----------------|---|
| input.sequences | ‘character’ vector. Sequences (uppercase single-letter code). |
| mode | Either “onehot”, “property”, or “geometric”. |
| property.set | Character string (one of the supported names) Defaults to “atchleyFactors”, but includes: “crucianiProperties”, “FASGAI”, “kideraFactors”, “MSWHIM”, “ProtFP”, “stScales”, “tScales”, “VHSE”, “zScales” Ignored if ‘property.matrix’ is supplied. |
| property.matrix | *Optional numeric matrix (‘20 × P’)*. Overrides ‘property.set’ in “property” mode. |

| | |
|---------------------|---|
| method | *(For geometric mode)* Character key for a built-in substitution matrix (e.g., "BLOSUM62"), or a 20x20 numeric matrix itself. |
| theta | *(For geometric mode)* Rotation angle in radians (default 'pi/3'). |
| sequence.dictionary | Character vector of the alphabet (default = 20 standard amino acids). |
| padding.symbol | Single character for right-padding (non-geometric modes). |
| summary.fun | For property mode only: "mean" or "" (none). |
| max.length | Integer for truncation/padding. If 'NULL' (default), the longest sequence sets the maximum. Not used in geometric mode. |
| nthreads | Number of threads for C++ backend. Not used in geometric mode. |
| verbose | Logical. If 'TRUE' (default), prints a progress message. |
| ... | Additional arguments passed to 'sequenceEncoder()' when using wrapper functions ('onehotEncoder', 'propertyEncoder', 'geometricEncoder'). |

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 | <i>Shannon Diversity Index (Entropy)</i> |
|-----------------|--|

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 *Fast Matrix Summaries*

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 <code>as.matrix()</code>). |
| 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): <ul style="list-style-type: none"> • "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> |

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