

Package ‘immApex’

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

Version 1.3.0

Description A set of tools to build tensorflow/keras3-based models 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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immApex-package	<i>immApex: Tools for Adaptive Immune Receptor Sequence-Based Machine and Deep Learning</i>
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Description

A set of tools to build tensorflow/keras3-based models 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)

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See Also

Useful links:

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

adjacencyMatrix	<i>Adjacency matrix from amino acid or nucleotide sequences</i>
-----------------	---

Description

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

Usage

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

Arguments

input.sequences	The amino acid or nucleotide sequences to use
normalize	Return the values as a function of total number of residues (TRUE) or frequencies (FALSE)
sequence.dictionary	The letters to use in sequence generation (default are all amino acids)

Value

Adjacency matrix based on input.sequences.

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)
```

buildNetwork	<i>Build Edit Distance Network Using Symmetric Deletion Lookup</i>
--------------	--

Description

Constructs a weighted similarity network from biological sequences using a symmetric deletion lookup strategy combined with a banded edit-distance computation. The returned igraph object contains vertices representing the input sequences and edges representing pairs of sequences whose edit distance is less than or equal to the specified threshold. The edge attribute weight stores the computed edit distance.

Usage

```
buildNetwork(
  input.data,
  sequence.column = "sequence",
  threshold = 2,
  filter.v = FALSE,
  filter.j = FALSE,
  technology = NULL,
  simplify.format = TRUE,
  simplify.families = TRUE
)
```

Arguments

<code>input.data</code>	A character vector of AIR sequences, or a data frame containing sequence data.
<code>sequence.column</code>	A character string specifying the name of the column in <code>input.data</code> that contains the sequences. Default is "sequence". This parameter is ignored when <code>input.data</code> is a character vector.
<code>threshold</code>	An integer specifying the maximum allowed edit distance. Only pairs of sequences with an edit distance less than or equal to this value will be connected. Default is 2.
<code>filter.v</code>	Logical indicating whether to filter candidate pairs to only those that have matching <code>v.gene</code> family annotations. Default is FALSE. When TRUE, the input data frame must contain a column with V gene annotations, either named <code>v.gene</code> or determined by <code>.get.genes.updated</code> .
<code>filter.j</code>	Logical indicating whether to filter candidate pairs to only those that have matching <code>j.gene</code> family annotations. Default is FALSE. When TRUE, the input data frame must contain a column with J gene annotations, either named <code>j.gene</code> or determined by <code>.get.genes.updated</code> .
<code>technology</code>	The sequencing technology employed - 'TenX', 'Adaptive', or 'AIRR'.
<code>simplify.format</code>	If applicable, remove the allelic designation (TRUE) or retain all information (FALSE)
<code>simplify.families</code>	If applicable, remove the hyphenated designation (TRUE) or retain all information (FALSE)

Details

This function supports both a character vector of sequences and a data frame. When provided a data frame, the user can specify the column containing sequences using the `sequence.column` parameter. Additionally, candidate pairs can be filtered by requiring matching `v.gene` and/or `j.gene` annotations (see `filter.v` and `filter.j`). If filtering is enabled, the corresponding gene annotation columns are required.

The function first calls a C++ routine (via Rcpp) to perform a symmetric deletion lookup, generating candidate pairs of sequences that might be within the specified edit distance. It then uses a banded dynamic programming algorithm (also implemented in C++) to compute the exact edit distance for each candidate pair. When using a data frame input, the candidate pairs can be further filtered by requiring that sequences have matching `v.gene` and/or `j.gene` values. Note that gene filtering is only applied if the corresponding filtering flag is set to TRUE.

Value

An igraph object representing the AIR similarity network. Vertices contain the original sequences (and gene annotations, if available), and each edge has a weight attribute corresponding to the computed edit distance. If no edges meet the threshold, an igraph object with only vertices is returned.

Examples

```
# Using a character vector of sequences:
sequences <- c("CASSLGTDQYF", "CASSPGTDQYF", "CASSLGNDQYF", "CASRLGNDQYF")
g <- buildNetwork(sequences, threshold = 2)
plot(g)

# Using a data frame with a custom sequence column:
df <- data.frame(
  mySeqs = c("CASSLGTDQYF", "CASSPGTDQYF", "CASSLGNDQYF", "CASRLGNDQYF"),
  v = c("TRBV20", "TRBV20", "TRBV12", "TRBV20"),
  j = c("TRBJ2-7", "TRBJ2-7", "TRBJ2-1", "TRBJ2-7")
)
g_df <- buildNetwork(df,
  threshold = 2,
  filter.v = TRUE,
  filter.j = TRUE,
  sequence.column = "mySeqs")
plot(g_df)
```

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 noise.

Usage

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

Arguments

prefix.motif Add defined amino acid/nucleotide sequence to the start of the generated sequences.

suffix.motif Add defined amino acid/nucleotide sequence to the end of the generated sequences

number.of.sequences Number of sequences to generate

min.length Minimum length of the final sequence. The min.length may be adjusted if incongruent with prefix.motif/suffix.motif lengths

max.length Maximum length of the final sequence

sequence.dictionary The letters to use in sequence generation (default are all amino acids)

Value

A vector of generated sequences

Examples

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

geometricEncoder

Geometric Encoder from Amino Acid Strings

Description

Use this to transform amino acid sequences into a geometric encoding of the sequence.

Usage

```
geometricEncoder(
  input.sequences,
  method.to.use = "BLOSUM62",
  theta = pi/3,
  verbose = TRUE
)
```

Arguments

input.sequences	The set of amino acid sequences
method.to.use	The method or approach for the conversion: • BLOcks SUBstitution Matrices: BLOSUM45, BLOSUM50, BLOSUM62, BLOSUM80, BLOSUM100 • Point Accepted Mutation Matrices: PAM30, PAM40, PAM70, PAM120, PAM250
theta	The angle for geometric transformation
verbose	Print messages corresponding to the processing step

Value

Geometric encoded amino acid sequences in a matrix

Examples

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

sequence.matrix <- geometricEncoder(new.sequences,
                                    method.to.use = "BLOSUM62",
                                    theta = pi/3)
```

getIMGT

Get IMGT Sequences for Specific Loci

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

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

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 = "aa")
```

Arguments

input.data	Single-cell object or the output of combineTCR and combineBCR from scRepertoire
chains	Immune Receptor chain to use - TRA , TRB , IGH , or IGL
sequence.type	Extract amino acid (aa) or nucleotide (nt) sequences

Value

A data frame of nucleotide or amino acid sequences

immapex_AA.data

*A list of amino acid properties***Description**

A list of amino acid properties that are used for [propertyEncoder](#) function.

This includes:

- atchleyFactors
- crucianiProperties
- FASGAI
- kideraFactors
- MSWHIM
- ProtFP
- stScales
- tScales
- VHSE
- zScales

Usage

```
data("immapex_AA.data")
```

Value

List of 10 amino acid properties for 20 amino acids

```
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 portions of the CDR Loop from Vgene data***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 = NULL,
  chain = "TRB",
  technology = NULL,
  sequence.type = "aa",
  sequences = c("CDR1", "CDR2")
)
```

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 , AIRR , or Omniscope
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 .

Value

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

Examples

```
# 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"))
```

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,  
    n.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
n.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,
                                     n.sequence = 1,
                                     position.start = 3,
                                     position.end = 8)
```

positionalEncoder	<i>Adding Position-Specific Information to Sequences</i>
-------------------	--

Description

Use this calculate positional encoding for recurrent neural networks using sin/cos and position information.

Usage

```
positionalEncoder(number.of.sequences, latent.dims = NULL)
```

Arguments

number.of.sequences	The number of sequences to generate position information
latent.dims	The number of latent dimensions.

Value

A matrix of values

Examples

```
position.info <- positionalEncoder(number.of.sequences = 1000,
                                   latent.dims = 64)
```

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

Description

Use this to generate a position-probability or weight matrix for a set of given sequences.

Usage

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

Arguments

input.sequences	The amino acid or nucleotide sequences to use
max.length	Additional length to pad, NULL will pad sequences to the max length of input.sequences
convert.PWM	Convert the matrix into a positional weight matrix using log likelihood
background.frequencies	Provide amino acid or nucleotide frequencies for the positional weight matrix. If NULL, assumes uniform likelihood.
sequence.dictionary	The letters to use in sequence generation (default are all amino acids)
padding.symbol	Symbol to use for padding at the end of sequences
verbose	Print messages corresponding to the processing step

Value

A matrix with position specific probabilities or weights

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)
```

propertyEncoder

Encoder from Amino Acid String by Properties

Description

Use this to transform amino acid sequences a a matrix by amino acid properties derived from dimensional reduction strategies

Usage

```
propertyEncoder(
  input.sequences,
  max.length = NULL,
  method.to.use = NULL,
  convert.to.matrix = TRUE,
  summary.function = NULL,
  padding.symbol = ".",
  verbose = TRUE
)
```

Arguments

<code>input.sequences</code>	The amino acid sequences to use
<code>max.length</code>	Additional length to pad, NULL will pad sequences to the max length of <code>input.sequences</code>
<code>method.to.use</code>	The method or approach to use for the conversion: • Individual sets: <code>atchleyFactors</code>, <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> • Multiple Sets: <code>c("atchleyFactors", "VHSE")</code>
<code>convert.to.matrix</code>	Return a matrix (TRUE) or a 3D array (FALSE)
<code>summary.function</code>	Return a matrix that summarize the amino acid method/property Available summaries include: "median", "mean", "sum", variance ("vars"), or Median Absolute Deviation ("mads")
<code>padding.symbol</code>	Symbol to use for padding at the end of sequences
<code>verbose</code>	Print messages corresponding to the processing step

Value

Converted amino acid sequences by property in a matrix or 3D array

Examples

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

if(reticulate::py_module_available("numpy")) {
  sequence.matrix <- propertyEncoder(new.sequences,
                                     method.to.use = "VHSE",
                                     convert.to.matrix = TRUE)
}
```

sequenceDecoder

One Hot Decoder from One Hot Encoded Matrix or 3D Array

Description

Use this to transform one hot encoded sequences back into amino acid or nucleotide sequences.

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,  
  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>verbose</code>	Print messages corresponding to the processing step

Value

Tokenize sequences in a matrix or vector

Examples

[illegible]

variationalSequences *Generate Similar Sequences using Variational Autoencoder*

Description

Use this to simulate sequences using a variational autoencoder (VAE) and perturbation of the probability distributions.

Usage

```
variationalSequences(
  input.sequences,
  encoder.function = "onehotEncoder",
  aa.method.to.use = NULL,
  number.of.sequences = 100,
  encoder.hidden.dim = c(128, 64),
  decoder.hidden.dim = NULL,
  latent.dim = 16,
  batch.size = 16,
  epochs = 50,
  learning.rate = 0.001,
  epsilon.std = 1,
  call.threshold = 0.2,
  activation.function = "relu",
  optimizer = "adam",
  disable.eager.execution = FALSE,
  sequence.dictionary = amino.acids,
  verbose = TRUE
)
```

Arguments

`input.sequences`
The amino acid or nucleotide sequences to use

`encoder.function`
The method to prepare the sequencing information - "onehotEncoder" or "propertyEncoder"

`aa.method.to.use`
The method or approach to use for the conversion:

- Individual sets: `atchleyFactors`, `crucianiProperties`, `FASGAI`, `kideraFactors`, `MSWHIM`, `ProtFP`, `stScales`, `tScales`, `VHSE`, `zScales`
- Multiple Sets: `c("atchleyFactors", "VHSE")`

`number.of.sequences`
Number of sequences to generate

`encoder.hidden.dim`
A vector of the neurons to use in the hidden layers for the encoder portion of the model

`decoder.hidden.dim`
A vector of the neurons to use in the hidden layers for the decoder portion of the model. If `NULL` assumes symmetric autoencoder

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