

Package ‘ttgsea’

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Type Package

Title Tokenizing Text of Gene Set Enrichment Analysis

Description Functional enrichment analysis methods such as gene set enrichment analysis (GSEA) have been widely used for analyzing gene expression data. GSEA is a powerful method to infer results of gene expression data at a level of gene sets by calculating enrichment scores for predefined sets of genes. GSEA depends on the availability and accuracy of gene sets. There are overlaps between terms of gene sets or categories because multiple terms may exist for a single biological process, and it can thus lead to redundancy within enriched terms. In other words, the sets of related terms are overlapping. Using deep learning, this package is aimed to predict enrichment scores for unique tokens or words from text in names of gene sets to resolve this overlapping set issue. Furthermore, we can coin a new term by combining tokens and find its enrichment score by predicting such a combined tokens.

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bi_gru	<i>Bidirectional GRU with embedding layer</i>
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Description

A predefined function that is used as a model in "ttgsea". This is a simple model, but you can define your own model. The loss function is "mean_squared_error" and the optimizer is "adam". Pearson correlation is used as a metric.

Usage

```
bi_gru(num_tokens, embedding_dim, length_seq, num_units)
```

Arguments

num_tokens	maximum number of tokens
embedding_dim	a non-negative integer for dimension of the dense embedding
length_seq	length of input sequences, input length of "layer_embedding"
num_units	dimensionality of the output space in the GRU layer

Value

model

Author(s)

Dongmin Jung

See Also

keras::keras_model, keras::layer_input, keras::layer_embedding, keras::layer_gru, keras::bidirectional, keras::layer_dense, keras::compile

Examples

```

library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  num_tokens <- 1000
  length_seq <- 30
  embedding_dim <- 50
  num_units <- 32
  model <- bi_gru(num_tokens, embedding_dim, length_seq, num_units)

  # stacked gru
  num_units_1 <- 32
  num_units_2 <- 16
  stacked_gru <- function(num_tokens, embedding_dim, length_seq,
                          num_units_1, num_units_2)
  {
    model <- keras::keras_model_sequential() %>%
      keras::layer_embedding(input_dim = num_tokens,
                            output_dim = embedding_dim,
                            input_length = length_seq,
                            mask_zero = TRUE) %>%
      keras::layer_gru(units = num_units_1,
                      activation = "relu",
                      return_sequences = TRUE) %>%
      keras::layer_gru(units = num_units_2,
                      activation = "relu") %>%
      keras::layer_dense(1)

    model %>%
      keras::compile(loss = "mean_squared_error",
                    optimizer = "adam",
                    metrics = custom_metric("pearson_correlation",
                                           metric_pearson_correlation))
  }
}

```

bi_lstm*Bidirectional LSTM with embedding layer*

Description

A predefined function that is used as a model in "ttgsea". This is a simple model, but you can define your own model. The loss function is "mean_squared_error" and the optimizer is "adam". Pearson correlation is used as a metric.

Usage

```
bi_lstm(num_tokens, embedding_dim, length_seq, num_units)
```

Arguments

num_tokens	maximum number of tokens
embedding_dim	a non-negative integer for dimension of the dense embedding
length_seq	length of input sequences, input length of "layer_embedding"
num_units	dimensionality of the output space in the LSTM layer

Value

model

Author(s)

Dongmin Jung

See Also

keras::keras_model, keras::layer_input, keras::layer_embedding, keras::layer_lstm, keras::bidirectional, keras::layer_dense, keras::compile

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  num_tokens <- 1000
  length_seq <- 30
  embedding_dim <- 50
  num_units <- 32
  model <- bi_lstm(num_tokens, embedding_dim, length_seq, num_units)

  # stacked lstm
  num_units_1 <- 32
  num_units_2 <- 16
  stacked_lstm <- function(num_tokens, embedding_dim, length_seq,
                           num_units_1, num_units_2)
  {
    model <- keras::keras_model_sequential() %>%
      keras::layer_embedding(input_dim = num_tokens,
                            output_dim = embedding_dim,
                            input_length = length_seq,
                            mask_zero = TRUE) %>%
      keras::layer_lstm(units = num_units_1,
                       activation = "relu",
                       return_sequences = TRUE) %>%
      keras::layer_lstm(units = num_units_2,
                       activation = "relu") %>%
      keras::layer_dense(1)

    model %>%
      keras::compile(loss = "mean_squared_error",
                    optimizer = "adam",
                    metrics = custom_metric("pearson_correlation",
                                           metric_pearson_correlation))
  }
}
```

Description

From the result of GSEA, we can predict enrichment scores for unique tokens or words from text in names of gene sets by using deep learning. The function "text_token" is used for tokenizing text and the function "token_vector" is used for encoding. Then the encoded sequence is fed to the embedding layer of the model.

Usage

```
fit_model(gseaRes, text, score, model, ngram_min = 1, ngram_max = 2,
          num_tokens, length_seq, epochs, batch_size,
          use_generator = TRUE, ...)
```

Arguments

gseaRes	a table with GSEA result having rows for gene sets and columns for text and scores
text	column name for text data
score	column name for enrichment score
model	deep learning model, input dimension and length for the embedding layer must be same to the "num_token" and "length_seq", respectively
ngram_min	minimum size of an n-gram (default: 1)
ngram_max	maximum size of an n-gram (default: 2)
num_tokens	maximum number of tokens, it must be equal to the input dimension of "layer_embedding" in the "model"
length_seq	length of input sequences, it must be equal to the input length of "layer_embedding" in the "model"
epochs	number of epochs
batch_size	batch size
use_generator	if "use_generator" is TRUE, the function "sampling_generator" is used for "fit_generator". Otherwise, the "fit" is used without a generator.
...	additional parameters for the "fit" or "fit_generator"

Value

model	trained model
tokens	information for tokens
token_pred	prediction for every token, each row has a token and its predicted score
token_gsea	list of the GSEA result only for the corresponding token
num_tokens	maximum number of tokens
length_seq	length of input sequences

Author(s)

Dongmin Jung

See Also

keras::fit_generator, keras::layer_embedding, keras::pad_sequences, textstem::lemmatize_strings, text2vec::create_vocabulary, text2vec::prune_vocabulary

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  library(fgsea)
  data(examplePathways)
  data(exampleRanks)
  names(examplePathways) <- gsub("_", " ",
                                substr(names(examplePathways), 9, 1000))

  set.seed(1)
  fgseaRes <- fgsea(examplePathways, exampleRanks)

  num_tokens <- 1000
  length_seq <- 30
  batch_size <- 32
  embedding_dims <- 50
  num_units <- 32
  epochs <- 1

  ttgseaRes <- fit_model(fgseaRes, "pathway", "NES",
                        model = bi_gru(num_tokens,
                                       embedding_dims,
                                       length_seq,
                                       num_units),
                        num_tokens = num_tokens,
                        length_seq = length_seq,
                        epochs = epochs,
                        batch_size = batch_size,
                        use_generator = FALSE)
}
```

metric_pearson_correlation

Pearson correlation coefficient

Description

Pearson correlation coefficient can be seen as one of the model performance metrics. This is a measure of how close the predicted value is to the true value. If it is close to 1, the model is considered a good fit. If it is close to 0, the model is not good. A value of 0 corresponds to a random prediction.

Author(s)

Dongmin Jung

See Also

keras::k_mean, keras::sum, keras::k_square, keras::k_sqrt

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  num_tokens <- 1000
  length_seq <- 30
  embedding_dims <- 50
  num_units_1 <- 32
  num_units_2 <- 16

  stacked_gru <- function(num_tokens, embedding_dims, length_seq,
                          num_units_1, num_units_2)
  {
    model <- keras::keras_model_sequential() %>%
      keras::layer_embedding(input_dim = num_tokens,
                             output_dim = embedding_dims,
                             input_length = length_seq) %>%
      keras::layer_gru(units = num_units_1,
                       activation = "relu",
                       return_sequences = TRUE) %>%
      keras::layer_gru(units = num_units_2,
                       activation = "relu") %>%
      keras::layer_dense(1)

    model %>%
      keras::compile(loss = "mean_squared_error",
                    optimizer = "adam",
                    metrics = custom_metric("pearson_correlation",
                                             metric_pearson_correlation))
  }
}
```

plot_model

visualization of the model architecture

Description

You are allowed to create a visualization of your model architecture. This architecture displays the information about the name, input shape, and output shape of layers in a flowchart.

Usage

```
plot_model(x)
```

Arguments

x deep learning model

Value

plot for the model architecture

Author(s)

Dongmin Jung

See Also

purrr::map, purrr::map_chr, purrr::pluck, purrr::imap_dfr, DiagrammeR::grViz

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  inputs1 <- layer_input(shape = c(1000))
  inputs2 <- layer_input(shape = c(1000))

  predictions1 <- inputs1 %>%
    layer_dense(units = 128, activation = 'relu') %>%
    layer_dense(units = 64, activation = 'relu') %>%
    layer_dense(units = 32, activation = 'softmax')

  predictions2 <- inputs2 %>%
    layer_dense(units = 128, activation = 'relu') %>%
    layer_dense(units = 64, activation = 'relu') %>%
    layer_dense(units = 32, activation = 'softmax')

  combined <- layer_concatenate(c(predictions1, predictions2)) %>%
    layer_dense(units = 16, activation = 'softmax')

  model <- keras_model(inputs = c(inputs1, inputs2),
                       outputs = combined)
  plot_model(model)
}
```

predict_model

Model prediction

Description

From the result of the function "ttgsea", we can predict enrichment scores. For each new term, lemmatized text, predicted enrichment score, Monte Carlo p-value and adjusted p-value are provided. The function "token_vector" is used for encoding as we did for training. Of course, mapping from tokens to integers should be the same.

Usage

```
predict_model(object, new_text, num_simulations = 1000,
              adj_p_method = "fdr")
```

Arguments

object	result of "ttgsea"
new_text	new text data
num_simulations	number of simulations for Monte Carlo p-value (default: 1000)
adj_p_method	correction method (default: "fdr")

Value

table for lemmatized text, predicted enrichment score, MC p-value and adjusted p-value

Author(s)

Dongmin Jung

See Also

stats::p.adjust

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  library(fgsea)
  data(examplePathways)
  data(exampleRanks)
  names(examplePathways) <- gsub("_", " ",
                                substr(names(examplePathways), 9, 1000))

  set.seed(1)
  fgseaRes <- fgsea(examplePathways, exampleRanks)

  num_tokens <- 1000
  length_seq <- 30
  batch_size <- 32
  embedding_dims <- 50
  num_units <- 32
  epochs <- 1

  ttgseaRes <- fit_model(fgseaRes, "pathway", "NES",
                        model = bi_gru(num_tokens,
                                       embedding_dims,
                                       length_seq,
                                       num_units),
                        num_tokens = num_tokens,
                        length_seq = length_seq,
                        epochs = epochs,
                        batch_size = batch_size,
                        use_generator = FALSE)

  set.seed(1)
  predict_model(ttgseaRes, "Cell Cycle")
}
```

sampling_generator

Generator function

Description

This is a generator function that yields batches of training data then pass the function to the "fit_generator" function.

Usage

```
sampling_generator(X_data, Y_data, batch_size)
```

Arguments

X_data	inputs
Y_data	targets
batch_size	batch size

Value

generator for "fit_generator"

Author(s)

Dongmin Jung

Examples

```
X_data <- matrix(rnorm(200), ncol = 2)
Y_data <- matrix(rnorm(100), ncol = 1)
sampling_generator(X_data, Y_data, 32)
```

text_token

Tokenizing text

Description

An n-gram is used for tokenization. This function can also be used to limit the total number of tokens.

Usage

```
text_token(text, ngram_min = 1, ngram_max = 1, num_tokens)
```

Arguments

text	text data
ngram_min	minimum size of an n-gram (default: 1)
ngram_max	maximum size of an n-gram (default: 1)
num_tokens	maximum number of tokens

Value

token	result of tokenizing text
ngram_min	minimum size of an n-gram
ngram_max	maximum size of an n-gram

Author(s)

Dongmin Jung

See Also

tm::removeWords, stopwords::stopwords, textstem::lemmatize_strings, text2vec::create_vocabulary, text2vec::prune_vocabulary

Examples

```
library(fgsea)
data(examplePathways)
data(exampleRanks)
names(examplePathways) <- gsub("_", " ",
                               substr(names(examplePathways), 9, 1000))
set.seed(1)
fgseaRes <- fgsea(examplePathways, exampleRanks)
tokens <- text_token(data.frame(fgseaRes)[,"pathway"],
                      num_tokens = 1000)
```

token_vector	<i>Vectorization of tokens</i>
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Description

A vectorization of words or tokens of text is necessary for machine learning. Vectorized sequences are padded or truncated.

Usage

```
token_vector(text, token, length_seq)
```

Arguments

text	text data
token	result of tokenization (output of "text_token")
length_seq	length of input sequences

Value

sequences of integers

Author(s)

Dongmin Jung

See Also

tm::removeWords, stopwords::stopwords, textstem::lemmatize_strings, tokenizers::tokenize_ngrams, keras::pad_sequences

Examples

```
library(reticulate)
if (keras::is_keras_available() & reticulate::py_available()) {
  library(fgsea)
  data(examplePathways)
  data(exampleRanks)
  names(examplePathways) <- gsub("_", " ",
                                substr(names(examplePathways), 9, 1000))
  set.seed(1)
  fgseaRes <- fgsea(examplePathways, exampleRanks)
  tokens <- text_token(data.frame(fgseaRes)[,"pathway"],
                       num_tokens = 1000)
  sequences <- token_vector("Cell Cycle", tokens, 10)
}
```

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