Package 'LBDiscover'

June 16, 2025

Title Literature-Based Discovery Tools for Biomedical Research

```
Version 0.1.0
Date 2025-06-12
Description A suite of tools for literature-based discovery in biomedical research.
      Provides functions for retrieving scientific articles from 'PubMed' and
      other NCBI databases, extracting biomedical entities (diseases, drugs, genes, etc.),
      building co-occurrence networks, and applying various discovery models
      including 'ABC', 'AnC', 'LSI', and 'BITOLA'. The package also includes
      visualization tools for exploring discovered connections.
License GPL-3
URL https://github.com/chaoliu-cl/LBDiscover,
      https://liu-chao.site/LBDiscover/
BugReports https://github.com/chaoliu-cl/LBDiscover/issues
Encoding UTF-8
RoxygenNote 7.3.2
Depends R (>= 4.1.0)
Imports httr (>= 1.4.0), xml2 (>= 1.3.0), igraph (>= 1.2.0), Matrix
      (>= 1.3.0), utils, stats, grDevices, graphics, tools, rentrez
      (>= 1.2.0), jsonlite (>= 1.7.0)
Suggests openxlsx (>= 4.2.0), SnowballC (>= 0.7.0), visNetwork (>=
      2.1.0), spacyr (>= 1.2.0), parallel, digest (>= 0.6.0), irlba
      (>= 2.3.0), knitr, rmarkdown, base64enc, reticulate, testthat
      (>= 3.0.0), mockery, covr, htmltools, data.table, tibble
Config/testthat/edition 3
NeedsCompilation no
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Repository CRAN
Date/Publication 2025-06-16 10:50:02 UTC
```

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Description

This function implements the ABC model for literature-based discovery with enhanced term filtering and validation.

```
abc_model(
  co_matrix,
  a_term,
  c_term = NULL,
  min_score = 0.1,
  n_results = 100,
```

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```
scoring_method = c("multiplication", "average", "combined", "jaccard"),
b_term_types = NULL,
c_term_types = NULL,
exclude_general_terms = TRUE,
filter_similar_terms = TRUE,
similarity_threshold = 0.8,
enforce_strict_typing = TRUE,
validation_method = "pattern"
)
```

Arguments

co_matrix A co-occurrence matrix produced by create_comat(). a_term Character string, the source term (A). Character string, the target term (C). If NULL, all potential C terms will be c_term evaluated. Minimum score threshold for results. min_score Maximum number of results to return. n_results scoring_method Method to use for scoring. Character vector of entity types allowed for B terms. b_term_types Character vector of entity types allowed for C terms. c_term_types exclude_general_terms Logical. If TRUE, excludes common general terms. filter_similar_terms Logical. If TRUE, filters out B-terms that are too similar to A-term. similarity_threshold Numeric. Maximum allowed string similarity between A and B terms. enforce_strict_typing Logical. If TRUE, enforces stricter entity type validation. validation_method Character. Method to use for entity validation: "pattern", "nlp", "api", or "com-

Value

A data frame with ranked discovery results.

prehensive".

abc_model_opt Optimize ABC model calculations for large matrices

Description

This function implements an optimized version of the ABC model calculation that's more efficient for large co-occurrence matrices.

abc_model_sig 5

Usage

```
abc_model_opt(
  co_matrix,
  a_term,
  c_term = NULL,
  min_score = 0.1,
  n_results = 100,
  chunk_size = 500
)
```

Arguments

co_matrix	A co-occurrence matrix produced by create_cooccurrence_matrix().
a_term	Character string, the source term (A).
c_term	Character string, the target term (C). If NULL, all potential C terms will be evaluated.
min_score	Minimum score threshold for results.
n_results	Maximum number of results to return.
chunk_size	Number of B terms to process in each chunk.

Value

A data frame with ranked discovery results.

abc_model_sig

Apply the ABC model with statistical significance testing

Description

This function extends the ABC model with statistical significance testing to evaluate the strength of discovered connections.

```
abc_model_sig(
  co_matrix,
  a_term,
  c_term = NULL,
  a_type = NULL,
  c_type = NULL,
  min_score = 0.1,
  n_results = 100,
  n_permutations = 1000,
  scoring_method = c("multiplication", "average", "combined", "jaccard")
)
```

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Arguments

co_matrix	A co-occurrence matrix produced by create_cooccurrence_matrix().
a_term	Character string, the source term (A).
c_term	Character string, the target term (C). If NULL, all potential C terms will be evaluated.
a_type	Character string, the entity type for A terms. If NULL, all types are considered.
c_type	Character string, the entity type for C terms. If NULL, all types are considered.
min_score	Minimum score threshold for results.
n_results	Maximum number of results to return.
$n_permutations$	Number of permutations for significance testing.
scoring_method	Method to use for scoring ABC connections.

Value

A data frame with ranked discovery results and p-values.

abc_timeslice	Apply time-sliced ABC model for validation	

Description

This function implements a time-sliced ABC model for validation. It uses historical data to predict connections that will appear in the future.

Usage

```
abc_timeslice(
  entity_data,
  time_column = "publication_year",
  split_time,
  a_term,
  a_type = NULL,
  c_type = NULL,
  min_score = 0.1,
  n_results = 100
)
```

Arguments

```
entity_data A data frame of entity data with time information.

time_column Name of the column containing time information.

split_time Time point to split historical and future data.

a_term Character string, the source term (A).
```

anc_model 7

a_type	Character string, the entity type for A terms.
c_type	Character string, the entity type for C terms.
min_score	Minimum score threshold for results.
n_results	Maximum number of results to return.

Value

A list with prediction results and validation metrics.

anc_model	ANC model for literature-based discovery with biomedical term filtering
-----------	---

Description

This function implements an improved ANC model that ensures only biomedical terms are used as intermediaries.

Usage

Arguments

```
co_matrix
                  A co-occurrence matrix produced by create_cooccurrence_matrix().
                  Character string, the source term (A).
a_term
n_b_terms
                  Number of intermediate B terms to consider.
                  Character string, the entity type for C terms. If NULL, all types are considered.
c_type
min_score
                  Minimum score threshold for results.
                  Maximum number of results to return.
n_results
enforce_biomedical_terms
                  Logical. If TRUE, enforces strict biomedical term filtering.
                  Character vector of entity types allowed for B terms.
b_term_types
validation_function
```

Function to validate biomedical terms.

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Value

A data frame with ranked discovery results.

bitola_model

Apply BITOLA-style discovery model

Description

This function implements a BITOLA-style discovery model based on MeSH term co-occurrence and semantic type filtering.

Usage

```
bitola_model(
   co_matrix,
   a_term,
   a_semantic_type = NULL,
   c_semantic_type = NULL,
   min_score = 0.1,
   n_results = 100
)
```

Arguments

```
co_matrix A co-occurrence matrix produced by create_cooccurrence_matrix().

a_term Character string, the source term (A).

a_semantic_type Character string, the semantic type for A term.

c_semantic_type Character string, the semantic type for C terms.

min_score Minimum score threshold for results.

n_results Maximum number of results to return.
```

Value

A data frame with ranked discovery results.

calc_bibliometrics 9

calc_bibliometrics

Calculate basic bibliometric statistics

Description

This function calculates basic bibliometric statistics from article data.

Usage

```
calc_bibliometrics(article_data, by_year = TRUE)
```

Arguments

article_data A data frame containing article data.

by_year Logical. If TRUE, calculates statistics by year.

Value

A list containing bibliometric statistics.

calc_doc_sim

Calculate document similarity using TF-IDF and cosine similarity

Description

This function calculates the similarity between documents using TF-IDF weighting and cosine similarity.

Usage

```
calc_doc_sim(
  text_data,
  text_column = "abstract",
  min_term_freq = 2,
  max_doc_freq = 0.9
)
```

Arguments

text_data A data frame containing text data.

text_column Name of the column containing text to analyze.
min_term_freq Minimum frequency for a term to be included.

max_doc_freq Maximum document frequency (as a proportion) for a term to be included.

Value

A similarity matrix for the documents.

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clear_pubmed_cache

Clear PubMed cache

Description

Removes all cached PubMed search results

Usage

```
clear_pubmed_cache()
```

Value

NULL invisibly

cluster_docs

Cluster documents using K-means

Description

This function clusters documents using K-means based on their TF-IDF vectors.

Usage

```
cluster_docs(
  text_data,
  text_column = "abstract",
  n_clusters = 5,
  min_term_freq = 2,
  max_doc_freq = 0.9,
  random_seed = 42
)
```

Arguments

text_data A data frame containing text data.

min_term_freq Minimum frequency for a term to be included.

max_doc_freq Maximum document frequency (as a proportion) for a term to be included.

random_seed Seed for random number generation (for reproducibility).

Value

A data frame with the original data and cluster assignments.

compare_terms 11

compare_terms

Compare term frequencies between two corpora

Description

This function compares term frequencies between two sets of articles.

Usage

```
compare_terms(
  corpus1,
  corpus2,
  text_column = "abstract",
  corpus1_name = "Corpus1",
  corpus2_name = "Corpus2",
  n = 100,
  remove_stopwords = TRUE
)
```

Arguments

corpus1 First corpus (data frame).

corpus2 Second corpus (data frame).

text_column Name of the column containing the text to analyze.

corpus1_name Name for the first corpus in the output.

corpus2_name Name for the second corpus in the output.

n Number of top terms to return.

remove_stopwords

Logical. If TRUE, removes stopwords.

Value

A data frame containing term frequency comparisons.

create_citation_net
Create a citation network from article data

Description

This function creates a citation network from article data. Note: Currently a placeholder as it requires citation data not available through basic PubMed queries.

```
create_citation_net(article_data, citation_data = NULL)
```

12 create_comat

Arguments

```
article_data A data frame containing article data.
citation_data A data frame containing citation data (optional).
```

Value

An igraph object representing the citation network.

create_comat

Create co-occurrence matrix without explicit entity type constraints

Description

This function creates a co-occurrence matrix from entity data while preserving entity type information as an attribute without enforcing type constraints.

Usage

```
create_comat(
  entity_data,
  doc_id_col = "doc_id",
  entity_col = "entity",
  count_col = NULL,
  type_col = "entity_type",
  normalize = TRUE,
  normalization_method = c("cosine", "jaccard", "dice")
)
```

Arguments

```
entity_data A data frame with document IDs and entities.

doc_id_col Name of the column containing document IDs.

entity_col Name of the column containing entity names.

count_col Name of the column containing entity counts (optional).

type_col Name of the column containing entity types (optional).

normalize Logical. If TRUE, normalizes the co-occurrence matrix.

normalization_method Method for normalization ("cosine", "jaccard", or "dice").
```

Value

A co-occurrence matrix with entity types stored as an attribute.

create_report 13

create_report

Generate a comprehensive discovery report

Description

This function generates an HTML report summarizing discovery results without enforcing entity type constraints. It includes data validation to avoid errors with publication years and other data issues.

Usage

```
create_report(
  results,
  visualizations = NULL,
  articles = NULL,
  output_file = "discovery_report.html"
)
```

Arguments

results A list containing discovery results from different approaches. visualizations A list containing file paths to visualizations.

articles A data frame containing the original articles.

output_file File path for the output HTML report.

Value

The file path of the created HTML report (invisibly).

create_sparse_comat

Create a sparse co-occurrence matrix

Description

This function creates a sparse co-occurrence matrix from entity data, which is more memory-efficient for large datasets.

```
create_sparse_comat(
  entity_data,
  doc_id_col = "doc_id",
  entity_col = "entity",
  count_col = NULL,
  type_col = NULL,
  normalize = TRUE
)
```

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Arguments

entity_data	A data frame with document IDs and entities.
doc_id_col	Name of the column containing document IDs.
entity_col	Name of the column containing entity names.
count_col	Name of the column containing entity counts (optional).
type_col	Name of the column containing entity types (optional).
normalize	Logical. If TRUE, normalizes the co-occurrence matrix.

Value

A sparse matrix of entity co-occurrences.

create_tdm	create_tdm	Create a term-document matrix from preprocessed text	
------------	------------	--	--

Description

This function creates a term-document matrix from preprocessed text data.

Usage

```
create_tdm(preprocessed_data, min_df = 2, max_df = 0.9)
```

Arguments

preprocessed_data

A data frame with preprocessed text data.

min_df Minimum document frequency for a term to be included.

max_df Maximum document frequency (as a proportion) for a term to be included.

Value

A term-document matrix.

create_term_document_matrix

Create a term-document matrix from preprocessed text

Description

This function creates a term-document matrix from preprocessed text data. It's a simplified version of create_tdm() for direct use in models.

Usage

```
create_term_document_matrix(preprocessed_data, min_df = 2, max_df = 0.9)
```

Arguments

preprocessed_data

A data frame with preprocessed text data.

min_df Minimum document frequency for a term to be included.

max_df Maximum document frequency (as a proportion) for a term to be included.

Value

A term-document matrix.

detect_lang

Detect language of text

Description

This function attempts to detect the language of a text string. It implements a simple n-gram based approach that doesn't require additional packages.

Usage

```
detect_lang(text, sample_size = 1000)
```

Arguments

text Text string to analyze

sample_size Maximum number of characters to sample for language detection

Value

Character string containing the ISO 639-1 language code

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diversify_abc

Enforce diversity in ABC model results

Description

This function applies diversity enforcement to ABC model results by:

- 1. Removing duplicate paths to the same C term
- 2. Ensuring B term diversity by selecting top results from each B term group
- 3. Preventing A and C terms from appearing as B terms

Usage

```
diversify_abc(
  abc_results,
  diversity_method = c("both", "b_term_groups", "unique_c_paths"),
  max_per_group = 3,
  min_score = 0.1
)
```

Arguments

```
abc_results A data frame containing ABC results.

diversity_method Method for enforcing diversity: "b_term_groups", "unique_c_paths", or "both".

max_per_group Maximum number of results to keep per B term or C term.

min_score Minimum score threshold for including connections.
```

Value

A data frame with diverse ABC results.

enhance_abc_kb

Enhance ABC results with external knowledge

Description

This function enhances ABC results with information from external knowledge bases.

```
enhance_abc_kb(abc_results, knowledge_base = c("umls", "mesh"), api_key = NULL)
```

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Arguments

```
abc_results A data frame containing ABC results.

knowledge_base Character string, the knowledge base to use ("umls" or "mesh").

api_key Character string. API key for the knowledge base (if needed).
```

Value

A data frame with enhanced ABC results.

eval_evidence Evaluate literature support for discovery results	
---	--

Description

This function evaluates the top results by searching for supporting evidence in the literature for the connections.

Usage

```
eval_evidence(
  results,
  max_results = 5,
  base_term = NULL,
  max_articles = 5,
  verbose = TRUE
)
```

Arguments

results The results to evaluate

max_results Maximum number of results to evaluate (default: 5)

base_term The base term for direct connection queries (e.g., "migraine")

max_articles Maximum number of articles to retrieve per search (default: 5)

verbose Logical; if TRUE, print evaluation results (default: TRUE)

Value

A list containing evaluation results

 ${\sf export_chord}$

Export interactive HTML chord diagram for ABC connections

Description

This function creates an HTML chord diagram visualization for ABC connections.

Usage

```
export_chord(
  abc_results,
  output_file = "abc_chord.html",
  top_n = 50,
  min_score = 0.1,
  open = TRUE
)
```

Arguments

abc_results A data frame containing ABC results.

output_file File path for the output HTML file.

top_n Number of top results to visualize.

min_score Minimum score threshold for including connections.

open Logical. If TRUE, opens the HTML file after creation.

Value

The file path of the created HTML file (invisibly).

 ${\tt export_chord_diagram} \quad \textit{Export interactive HTML chord diagram for ABC connections}$

Description

This function creates an HTML chord diagram visualization for ABC connections, properly coloring the arcs based on whether each term is an A, B, or C term.

```
export_chord_diagram(
  abc_results,
  output_file = "abc_chord.html",
  top_n = 50,
  min_score = 0.1,
  open = TRUE,
  layout_seed = NULL
)
```

export_network 19

Arguments

abc_results A data frame containing ABC results.

output_file File path for the output HTML file.

top_n Number of top results to visualize.

min_score Minimum score threshold for including connections.

open Logical. If TRUE, opens the HTML file after creation.

layout_seed Optional seed for layout reproducibility. If NULL, no seed is set.

Value

The file path of the created HTML file (invisibly).

export_network

Export ABC results to simple HTML network

Description

This function exports ABC results to a simple HTML file with a visualization. If the visNetwork package is available, it will use it for a more interactive visualization.

Usage

```
export_network(
  abc_results,
  output_file,
  top_n = 50,
  min_score = 0.1,
  open = TRUE
)
```

Arguments

abc_results A data frame containing ABC results from apply_abc_model().

output_file File path for the output HTML file. Must be specified by user.

top_n Number of top results to visualize.

min_score Minimum score threshold for including connections.

open Logical. If TRUE, opens the HTML file after creation.

Value

The file path of the created HTML file (invisibly).

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Examples

```
# Create sample ABC results
abc_results <- data.frame(
   a_term = rep("migraine", 3),
   b_term = c("serotonin", "dopamine", "noradrenaline"),
   c_term = c("sumatriptan", "ergotamine", "propranolol"),
   a_b_score = c(0.8, 0.7, 0.6),
   b_c_score = c(0.9, 0.8, 0.7),
   abc_score = c(0.72, 0.56, 0.42)
)

# Export to temporary file
temp_file <- file.path(tempdir(), "network.html")
export_network(abc_results, temp_file, open = FALSE)

# Clean up
unlink(temp_file)</pre>
```

extract_entities

Extract and classify entities from text with multi-domain types

Description

This function extracts entities from text and optionally assigns them to specific semantic categories based on dictionaries.

Usage

```
extract_entities(
  text_data,
  text_column = "abstract",
  dictionary = NULL,
  case_sensitive = FALSE,
  overlap_strategy = c("priority", "all", "longest"),
  sanitize_dict = TRUE
)
```

Arguments

```
text_data A data frame containing article text data.

text_column Name of the column containing text to process.

dictionary Combined dictionary or list of dictionaries for entity extraction.

case_sensitive Logical. If TRUE, matching is case-sensitive.

overlap_strategy

How to handle terms that match multiple dictionaries: "priority", "all", or "longest".

sanitize_dict Logical. If TRUE, sanitizes the dictionary before extraction.
```

Value

A data frame with extracted entities, their types, and positions.

```
extract_entities_workflow
```

Extract entities from text with improved efficiency using only base R

Description

This function provides a complete workflow for extracting entities from text using dictionaries from multiple sources, with improved performance and robust error handling.

Usage

```
extract_entities_workflow(
  text_data,
  text_column = "abstract",
  entity_types = c("disease", "drug", "gene"),
  dictionary_sources = c("local", "mesh", "umls"),
  additional_mesh_queries = NULL,
  sanitize = TRUE,
  api_key = NULL,
  custom_dictionary = NULL,
 max_terms_per_type = 200,
  verbose = TRUE,
  batch_size = 500,
  parallel = FALSE,
  num\_cores = 2,
  cache_dictionaries = TRUE
)
```

Arguments

A data frame containing custom dictionary entries to incorporate into the entity extraction process.

22 extract_ner

```
max_terms_per_type
```

Maximum number of terms to fetch per entity type. Default is 200.

verbose Logical. If TRUE, prints detailed progress information.

batch_size Number of documents to process in a single batch. Default is 500.

parallel Logical. If TRUE, uses parallel processing when available. Default is FALSE.

num_cores Number of cores to use for parallel processing. Default is 2.

cache_dictionaries

Logical. If TRUE, caches dictionaries for faster reuse. Default is TRUE.

Value

A data frame with extracted entities, their types, and positions.

extract_ner

Perform named entity recognition on text

Description

This function performs a simple dictionary-based named entity recognition. For more advanced NER, consider using external tools via reticulate.

Usage

```
extract_ner(
  text,
  entity_types = c("disease", "drug", "gene"),
  custom_dictionaries = NULL
)
```

Arguments

text Character vector of texts to process

entity_types Character vector of entity types to recognize

custom_dictionaries

List of custom dictionaries (named by entity type)

Value

A data frame containing found entities, their types, and positions

extract_ngrams 23

ovtract	narome	
extract	ngrams	

Extract n-grams from text

Description

This function extracts n-grams (sequences of n words) from text.

Usage

```
extract_ngrams(text, n = 1, min_freq = 2)
```

Arguments

text Character vector of texts to process

n Integer specifying the n-gram size (1 for unigrams, 2 for bigrams, etc.)

min_freq Minimum frequency to include an n-gram

Value

A data frame containing n-grams and their frequencies

extract_terms

Extract common terms from a corpus

Description

This function extracts and counts the most common terms in a corpus.

Usage

```
extract_terms(
  article_data,
  text_column = "abstract",
  n = 100,
  remove_stopwords = TRUE,
  min_word_length = 3
)
```

Arguments

```
article_data A data frame containing article data.

text_column Name of the column containing the text to analyze.

n Number of top terms to return.

remove_stopwords

Logical. If TRUE, removes stopwords.

min_word_length
```

Minimum word length to include.

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Value

A data frame containing term counts.

extract_topics

Apply topic modeling to a corpus

Description

This function implements a simple non-negative matrix factorization (NMF) approach to topic modeling, without requiring additional packages.

Usage

```
extract_topics(
  text_data,
  text_column = "abstract",
  n_topics = 5,
  max_terms = 10,
  n_iterations = 50,
  seed = NULL
)
```

Arguments

text_data A data frame containing the text data

text_column Name of the column containing the text

n_topics Number of topics to extract

max_terms Maximum number of terms per topic to return

n_iterations Number of iterations for the NMF algorithm

seed Optional seed for reproducibility. If NULL, no seed is set.

Value

A list containing topic-term and document-topic matrices

filter_by_type 25

filter_by_type	Filter a co-occurrence matrix by entity type
----------------	--

Description

Filter a co-occurrence matrix by entity type

Usage

```
filter_by_type(co_matrix, types)
```

Arguments

co_matrix A co-occurrence matrix produced by create_typed_comat().
types Character vector of entity types to include.

Value

A filtered co-occurrence matrix.

find_abc_all	Find all potential ABC connections
--------------	------------------------------------

Description

This function finds all potential ABC connections in a co-occurrence matrix.

Usage

```
find_abc_all(
  co_matrix,
  a_type = NULL,
  c_type = NULL,
  min_score = 0.1,
  n_results = 1000
)
```

Arguments

co_matrix	A co-occurrence matrix produced by create_comat().
a_type	Character string, the entity type for A terms.
c_type	Character string, the entity type for C terms.
min_score	Minimum score threshold for results.
n_results	Maximum number of results to return.

26 find_term

Value

A data frame with ranked discovery results.

find_similar_docs Find similar documents for a given document	
---	--

Description

This function finds documents similar to a given document based on TF-IDF and cosine similarity.

Usage

```
find_similar_docs(text_data, doc_id, text_column = "abstract", n_similar = 5)
```

Arguments

text_data A data frame containing text data.

doc_id ID of the document to find similar documents for. text_column Name of the column containing text to analyze.

n_similar Number of similar documents to return.

Value

A data frame with similar documents and their similarity scores.

find_term	Find primary term in co-occurrence matrix	

Description

This function verifies that the primary term exists in the co-occurrence matrix, and if not, attempts to find a suitable variation.

Usage

```
find_term(co_matrix, primary_term, verbose = TRUE)
```

Arguments

co_matrix The co-occurrence matrix primary_term The primary term to find

verbose Logical; if TRUE, print status messages (default: TRUE)

Value

The found term (either exact match or variation)

gen_report 27

gen_report	Generate comprehensive discovery report
------------	---

Description

This function creates a comprehensive HTML report from discovery results and visualizations.

Usage

```
gen_report(
  results_list,
  visualizations = NULL,
  articles = NULL,
  output_file = "discoveries.html",
  verbose = TRUE
)
```

Arguments

results_list A list of result data frames from different approaches

visualizations A list with paths to visualization files

articles Prepared article data

output_file Filename for the output HTML report

verbose Logical; if TRUE, print status messages (default: TRUE)

Value

Invisible output_file path

get_dict_cache Get dictionary cache environment

Description

Get dictionary cache environment

Usage

```
get_dict_cache()
```

Value

The environment containing cached dictionary data

28 get_term_vars

get	nmc	ful	1	text
5 C L_	_DIIIC_	_ 1 4 4		ししへし

Retrieve full text from PubMed Central

Description

This function retrieves full text articles from PubMed Central.

Usage

```
get_pmc_fulltext(pmids, api_key = NULL)
```

Arguments

pmids Character vector of PubMed IDs.

api_key Character string. NCBI API key for higher rate limits (optional).

Value

A data frame containing article metadata and full text.

get_term_vars

Extract term variations from text corpus

Description

This function identifies variations of a primary term within a corpus of articles.

Usage

```
get_term_vars(articles, primary_term, text_col = "abstract")
```

Arguments

articles A data frame containing article data with text columns

primary_term The primary term to find variations of

text_col Name of the column containing the text to search

Value

A character vector of unique term variations, sorted by length

get_type_dist 29

get_type_dist

Get entity type distribution from co-occurrence matrix

Description

Get entity type distribution from co-occurrence matrix

Usage

```
get_type_dist(co_matrix)
```

Arguments

co_matrix

A co-occurrence matrix produced by create_typed_comat().

Value

A data frame with entity type counts and percentages.

```
is_valid_biomedical_entity
```

Determine if a term is likely a specific biomedical entity with improved accuracy

Description

Determine if a term is likely a specific biomedical entity with improved accuracy

Usage

```
is_valid_biomedical_entity(term, claimed_type = NULL)
```

Arguments

term Character string, the term to check

claimed_type Character string, the claimed entity type of the term

Value

Logical, TRUE if the term is likely a valid biomedical entity, FALSE otherwise

30 load_dictionary

load_dictionary Load biomedical dictionaries with improved error handling

Description

This function loads pre-defined biomedical dictionaries or fetches terms from MeSH/UMLS.

Usage

```
load_dictionary(
  dictionary_type = NULL,
  custom_path = NULL,
  source = c("local", "mesh", "umls"),
  api_key = NULL,
  n_terms = 200,
  mesh_query = NULL,
  semantic_type_filter = NULL,
  sanitize = TRUE,
  extended_mesh = FALSE,
  mesh_queries = NULL
)
```

Arguments

dictionary_type

Type of dictionary to load. For local dictionaries, limited to "disease", "drug",

"gene". For MeSH and UMLS, expanded to include more semantic categories.

custom_path Optional path to a custom dictionary file.

source The source to fetch terms from: "local", "mesh", or "umls".

api_key UMLS API key for authentication (required if source = "umls").

n_terms Number of terms to fetch.

mesh_query Additional query to filter MeSH terms (only if source = "mesh").

semantic_type_filter

Filter by semantic type (used mainly with UMLS).

sanitize Logical. If TRUE, sanitizes the dictionary terms.

extended_mesh Logical. If TRUE and source is "mesh", uses PubMed search for additional

terms

mesh_queries Named list of MeSH queries for different categories (only if extended_mesh =

TRUE).

Value

A data frame containing the dictionary.

load_results 31

load_results

Load saved results from a file

Description

This function loads previously saved results from a file.

Usage

```
load_results(file_path)
```

Arguments

file_path

File path to load the results from.

Value

A data frame containing the loaded results.

lsi_model

LSI model with enhanced biomedical term filtering and NLP verification

Description

This function implements an improved LSI model that more rigorously filters out non-biomedical terms from the results to ensure clinical relevance. It adds NLP-based validation as an additional layer of filtering.

```
lsi_model(
  term_doc_matrix,
  a_term,
  n_factors = 100,
  n_results = 100,
  enforce_biomedical_terms = TRUE,
  c_term_types = NULL,
  entity_types = NULL,
  validation_function = is_valid_biomedical_entity,
  min_word_length = 3,
  use_nlp = TRUE,
  nlp_threshold = 0.7
)
```

32 map_ontology

Arguments

```
term_doc_matrix
                  A term-document matrix.
a_term
                  Character string, the source term (A).
                  Number of factors to use in LSI.
n_factors
n_results
                  Maximum number of results to return.
enforce_biomedical_terms
                  Logical. If TRUE, enforces strict biomedical term filtering.
                  Character vector of entity types allowed for C terms.
c_term_types
entity_types
                  Named vector of entity types (if NULL, will try to detect).
validation_function
                  Function to validate biomedical terms.
min_word_length
                  Minimum word length to include.
use_nlp
                  Logical. If TRUE, uses NLP-based validation for biomedical terms.
```

Value

A data frame with ranked discovery results.

map_ontology

nlp_threshold

Map terms to biomedical ontologies

Numeric between 0 and 1. Minimum confidence for NLP validation.

Description

This function maps terms to standard biomedical ontologies like MeSH or UMLS.

```
map_ontology(
  terms,
  ontology = c("mesh", "umls"),
  api_key = NULL,
  fuzzy_match = FALSE,
  similarity_threshold = 0.8,
  mesh_query = NULL,
  semantic_types = NULL,
  dictionary_type = "disease"
)
```

merge_entities 33

Arguments

terms	Character vector of terms to map
ontology	Character string. The ontology to use: "mesh" or "umls"
api_key	UMLS API key (required if ontology = "umls")
<pre>fuzzy_match similarity_thre</pre>	Logical. If TRUE, allows fuzzy matching of terms eshold
	Numeric between 0 and 1. Minimum similarity for fuzzy matching
mesh_query	Additional query to filter MeSH terms (only if ontology = "mesh")
semantic_types	Vector of semantic types to filter UMLS results
dictionary_type	
	Type of dictionary to use ("disease", "drug", "gene", etc.)

Value

A data frame with mapped terms and ontology identifiers

merge_entities Combine and deduplicate entity datasets

Description

This function combines custom and standard entity datasets, handling the case where one or both might be empty, and removes duplicates.

Usage

```
merge_entities(
  custom_entities,
  standard_entities,
  primary_term,
  primary_type = "disease",
  verbose = TRUE
)
```

Arguments

```
custom_entities

Data frame of custom entities (can be NULL)

standard_entities

Data frame of standard entities (can be NULL)

primary_term

The primary term of interest

primary_type

The entity type of the primary term (default: "disease")

verbose

Logical; if TRUE, print status messages (default: TRUE)
```

Value

A data frame of combined entities

34 min_results

merge_results

Merge multiple search results

Description

This function merges multiple search results into a single data frame.

Usage

```
merge_results(..., remove_duplicates = TRUE)
```

Arguments

```
... Data frames containing search results.

remove_duplicates

Logical. If TRUE, removes duplicate articles.
```

Value

A merged data frame.

min_results

Ensure minimum results for visualization

Description

This function ensures there are sufficient results for visualization, creating placeholder data if necessary.

```
min_results(
   diverse_results,
   top_results,
   a_term,
   min_results = 3,
   fallback_count = 15,
   verbose = TRUE
)
```

ncbi_search 35

Arguments

diverse_results

Current diversified results

top_results Original top results

a_term The primary term for the analysis

min_results Minimum number of desired results (default: 3)
fallback_count Number of top results to use as fallback (default: 15)
verbose Logical; if TRUE, print status messages (default: TRUE)

Value

A data frame with sufficient results for visualization

ncbi_search

Search NCBI databases for articles or data

Description

This function searches various NCBI databases using the E-utilities API via the rentrez package.

Usage

```
ncbi_search(
  query,
  database = "pubmed",
  max_results = 1000,
  use_mesh = FALSE,
  date_range = NULL,
  api_key = NULL,
  retry_count = 3,
  retry_delay = 2
)
```

Arguments

query Character string containing the search query.

database Character string. The NCBI database to search (e.g., "pubmed", "pmc", "gene",

"protein").

max_results Maximum number of results to return.

use_mesh Logical. If TRUE, will attempt to map query terms to MeSH terms (for PubMed

only).

date_range Character vector of length 2 with start and end dates in format "YYYY/MM/DD".

api_key Character string. NCBI API key for higher rate limits (optional).

retry_count Integer. Number of times to retry failed requests.

retry_delay Integer. Delay between retries in seconds.

36 parallel_analysis

Value

A data frame containing the search results with IDs, titles, and other metadata.

parallel_analysis

Apply parallel processing for document analysis

Description

This function uses parallel processing to analyze documents faster.

Usage

```
parallel_analysis(
  text_data,
  analysis_function,
  text_column = "abstract",
  ...,
  n_cores = NULL
)
```

Arguments

text_data A data frame containing text data. analysis_function

Function to apply to each document.

text_column Name of the column containing text to analyze.

. . . Additional arguments passed to the analysis function.

n_cores Number of cores to use for parallel processing. If NULL, uses all available cores

minus 1.

Value

A data frame with analysis results.

perm_test_abc 37

perm_test_abc

Perform randomization test for ABC model

Description

This function assesses the significance of ABC model results through randomization. It generates a null distribution by permuting the co-occurrence matrix.

Usage

```
perm_test_abc(abc_results, co_matrix, n_permutations = 1000, alpha = 0.05)
```

Arguments

abc_results A data frame containing ABC results.

co_matrix The co-occurrence matrix used to generate the ABC results.

n_permutations Number of permutations to perform.

alpha Significance level.

Value

A data frame with ABC results and permutation-based significance measures.

plot_heatmap

Create heatmap visualization from results

Description

This function creates a heatmap visualization from ABC results.

```
plot_heatmap(
   results,
   output_file = "heatmap.png",
   width = 1200,
   height = 900,
   resolution = 120,
   top_n = 15,
   min_score = 1e-04,
   color_palette = "blues",
   show_entity_types = TRUE,
   verbose = TRUE
```

38 plot_network

Arguments

results The results to visualize output_file Filename for the output PNG (default: "heatmap.png") width Width of the output image (default: 1200) height Height of the output image (default: 900) resolution Resolution of the output image (default: 120) Maximum number of results to include (default: 15) top_n min_score Minimum score threshold (default: 0.0001) color_palette Color palette for the heatmap (default: "blues") show_entity_types Logical; if TRUE, show entity types (default: TRUE) Logical; if TRUE, print status messages (default: TRUE) verbose

Value

Invisible NULL (creates a file as a side effect)

plot_network

Create network visualization from results

Description

This function creates a network visualization from ABC results.

```
plot_network(
  results,
  output_file = "network.png",
  width = 1200,
  height = 900,
  resolution = 120,
  top_n = 15,
  min_score = 1e-04,
  node_size_factor = 5,
  color_by = "type",
  title = "Network Visualization",
  show_entity_types = TRUE,
  label_size = 1,
  verbose = TRUE
)
```

preprocess_text 39

Arguments

results The results to visualize

output_file Filename for the output PNG (default: "network.png")

width Width of the output image (default: 1200)
height Height of the output image (default: 900)

resolution Resolution of the output image (default: 120)

top_n Maximum number of results to include (default: 15)

min_score Minimum score threshold (default: 0.0001)

node_size_factor

Factor for scaling node sizes (default: 5)

color_by Column to use for node colors (default: "type")

title Plot title (default: "Network Visualization")

show_entity_types

Logical; if TRUE, show entity types (default: TRUE)

label_size Relative size for labels (default: 1.0)

verbose Logical; if TRUE, print status messages (default: TRUE)

Value

Invisible NULL (creates a file as a side effect)

Description

This function preprocesses article text for further analysis.

```
preprocess_text(
   text_data,
   text_column = "abstract",
   remove_stopwords = TRUE,
   custom_stopwords = NULL,
   stem_words = FALSE,
   min_word_length = 3,
   max_word_length = 50
)
```

40 prep_articles

Arguments

text_data A data frame containing article text data (title, abstract, etc.).

remove_stopwords

Logical. If TRUE, removes stopwords.

custom_stopwords

Character vector of additional stopwords to remove.

stem_words Logical. If TRUE, applies stemming to words.

min_word_length

Minimum word length to keep.

max_word_length

Maximum word length to keep.

Value

A data frame with processed text and extracted terms.

prep_articles

Prepare articles for report generation

Description

This function ensures article data is valid for report generation, particularly handling publication years.

Usage

```
prep_articles(articles, verbose = TRUE)
```

Arguments

articles The article data frame (can be NULL)

verbose Logical; if TRUE, print status messages (default: TRUE)

Value

A data frame of articles with validated publication years

pubmed_search 41

pubmed_search	Search PubMed for articles with optimized performance	

Description

This function searches PubMed using the NCBI E-utilities API via the rentrez package. The implementation includes optimizations for speed, memory efficiency, and reliability.

Usage

```
pubmed_search(
   query,
   max_results = 1000,
   use_mesh = FALSE,
   date_range = NULL,
   api_key = NULL,
   batch_size = 200,
   verbose = TRUE,
   use_cache = TRUE,
   retry_count = 3,
   retry_delay = 1
)
```

Arguments

query	Character string containing the search query.
max_results	Maximum number of results to return.
use_mesh	Logical. If TRUE, will attempt to map query terms to MeSH terms.
date_range	Character vector of length 2 with start and end dates in format "YYYY/MM/DD".
api_key	Character string. NCBI API key for higher rate limits (optional).
batch_size	Integer. Number of records to fetch in each batch (default: 200).
verbose	Logical. If TRUE, prints progress information.
use_cache	Logical. If TRUE, cache results to avoid redundant API calls.
retry_count	Integer. Number of times to retry failed API calls.
retry_delay	Integer. Initial delay between retries in seconds.

Value

A data frame containing the search results with PubMed IDs, titles, and other metadata.

42 query_mesh

query_external_api

Query external biomedical APIs to validate entity types

Description

Query external biomedical APIs to validate entity types

Usage

```
query_external_api(term, claimed_type)
```

Arguments

term Character string, the term to validate

claimed_type Character string, the claimed entity type

Value

Logical indicating if the term was found in the appropriate database

query_mesh

Query for MeSH terms using E-utilities

Description

Query for MeSH terms using E-utilities

Usage

```
query_mesh(term, api_key = NULL)
```

Arguments

term Character string, the term to query.

api_key Character string. NCBI API key (optional).

Value

A data frame with MeSH information for the term.

query_umls 43

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uucı v	ullit	

Query UMLS for term information

Description

Query UMLS for term information

Usage

```
query_umls(term, api_key, version = "current")
```

Arguments

term	Character string, the term to query.	
api_key	Character string. UMLS API key.	
version	Character string. UMLS version to use	

Value

A data frame with UMLS information for the term.

run_lbd	Perform comprehensive literature-based discovery without type con-
	straints

Description

This function performs a comprehensive literature-based discovery analysis using multiple approaches without enforcing entity type constraints.

```
run_lbd(
    search_query,
    a_term,
    max_results = 100,
    discovery_approaches = c("abc", "anc", "lsi", "bitola"),
    include_visualizations = TRUE,
    output_file,
    api_key = NULL,
    dictionary_sources = c("local", "mesh", "umls"),
    entity_categories = c("disease", "drug", "gene")
)
```

44 safe_diversify

Arguments

```
Character string, the search query for retrieving initial articles.
search_query
                  Character string, the source term (A) for discovery.
a_term
                  Maximum number of results to return for each approach.
max_results
discovery_approaches
                  Character vector, the discovery approaches to use.
include_visualizations
                  Logical. If TRUE, generates visualizations.
output_file
                  File path for the output report. Must be specified by user.
api_key
                  Character string. API key for PubMed and other services.
dictionary_sources
                  Character vector. Sources for entity dictionaries: "local", "mesh", "umls".
entity_categories
                  Character vector. Entity categories to include.
```

Value

A list containing discovery results from all approaches.

Examples

```
# Example with temporary output file
temp_report <- file.path(tempdir(), "discovery_report.html")

results <- run_lbd(
    search_query = "migraine treatment",
    a_term = "migraine",
    max_results = 10,
    discovery_approaches = "abc",
    include_visualizations = FALSE,
    output_file = temp_report
)

# Clean up
unlink(temp_report)
unlink(list.files(tempdir(), pattern = "*.png", full.names = TRUE))
unlink(list.files(tempdir(), pattern = "*.html", full.names = TRUE))</pre>
```

safe_diversify

Diversify ABC results with error handling

Description

This function diversifies ABC results to avoid redundancy, with error handling to ensure results are always returned.

sanitize_dictionary 45

Usage

```
safe_diversify(
  top_results,
  diversity_method = "both",
  max_per_group = 5,
  min_score = 1e-04,
  min_results = 5,
  fallback_count = 15,
  verbose = TRUE
)
```

Arguments

Value

A data frame of diversified results

```
sanitize_dictionary Enhanced sanitize dictionary function
```

Description

This function sanitizes dictionary terms to ensure they're valid for entity extraction.

```
sanitize_dictionary(
  dictionary,
  term_column = "term",
  type_column = "type",
  validate_types = TRUE,
  verbose = TRUE
)
```

46 save_results

Arguments

dictionary A data frame containing dictionary terms.

term_column The name of the column containing the terms to sanitize.

type_column The name of the column containing entity types.

validate_types Logical. If TRUE, validates terms against their claimed type.

verbose Logical. If TRUE, prints information about the filtering process.

Value

A data frame with sanitized terms.

save_results

Save search results to a file

Description

This function saves search results to a file.

Usage

```
save_results(results, file_path, format = c("csv", "rds", "xlsx"))
```

Arguments

results A data frame containing search results.

file_path File path to save the results. Must be specified by user. File format to use. One of "csv", "rds", or "xlsx".

Value

The file path (invisibly).

Examples

```
# Create sample results
results <- data.frame(
   pmid = c("12345", "67890"),
   title = c("Sample Title 1", "Sample Title 2"),
   abstract = c("Sample abstract 1", "Sample abstract 2")
)

# Save to temporary directory
temp_file <- file.path(tempdir(), "results.csv")
save_results(results, temp_file, format = "csv")

# Clean up
unlink(temp_file)</pre>
```

segment_sentences 47

segment_sentences

Perform sentence segmentation on text

Description

This function splits text into sentences.

Usage

```
segment_sentences(text)
```

Arguments

text

Character vector of texts to process

Value

A list where each element contains a character vector of sentences

validate_abc

Apply statistical validation to ABC model results with support for large matrices

Description

This function performs statistical tests to validate ABC model results. It calculates p-values using hypergeometric tests and applies correction for multiple testing. The function is optimized to work with very large co-occurrence matrices.

Usage

```
validate_abc(
  abc_results,
  co_matrix,
  alpha = 0.05,
  correction = c("BH", "bonferroni", "none"),
  filter_by_significance = FALSE
)
```

Arguments

abc_results A data frame containing ABC results.

co_matrix The co-occurrence matrix used to generate the ABC results.

alpha Significance level (p-value threshold). correction Method for multiple testing correction.

filter_by_significance

Logical. If TRUE, only returns significant results.

Value

A data frame with ABC results and statistical significance measures.

```
validate_biomedical_entity
```

Validate biomedical entities using BioBERT or other ML models

Description

Validate biomedical entities using BioBERT or other ML models

Usage

```
validate_biomedical_entity(term, claimed_type)
```

Arguments

```
term Character string, the term to validate claimed_type Character string, the claimed entity type
```

Value

Logical indicating if the term is validated

```
validate_entity_comprehensive
```

Comprehensive entity validation using multiple techniques

Description

Comprehensive entity validation using multiple techniques

```
validate_entity_comprehensive(
  term,
  claimed_type,
  use_nlp = TRUE,
  use_pattern = TRUE,
  use_external_api = FALSE
)
```

validate_entity_with_nlp

Arguments

term Character string, the term to validate
claimed_type Character string, the claimed entity type

use_nlp Logical, whether to use NLP-based validation

use_pattern Logical, whether to use pattern-based validation

use_external_api

Logical, whether to query external APIs

Value

Logical indicating if the term is validated

```
validate_entity_with_nlp
```

Validate entity types using NLP-based entity recognition with improved accuracy

Description

Validate entity types using NLP-based entity recognition with improved accuracy

Usage

```
validate_entity_with_nlp(term, claimed_type, nlp_model = NULL)
```

Arguments

term Character string, the term to validate
claimed_type Character string, the claimed entity type
nlp_model The loaded NLP model to use for validation

Value

Logical indicating if the term is likely of the claimed type

valid_entities

validate_umls_key

Validate a UMLS API key

Description

This function validates a UMLS API key using the validation endpoint.

Usage

```
validate_umls_key(api_key, validator_api_key = NULL)
```

Arguments

```
api_key UMLS API key to validate
validator_api_key
Your application's UMLS API key (for third-party validation)
```

Value

Logical indicating if the API key is valid

valid_entities

Filter entities to include only valid biomedical terms

Description

This function applies validation to ensure only legitimate biomedical entities are included, while preserving trusted terms.

```
valid_entities(
  entities,
  primary_term,
  primary_term_variations = NULL,
  validation_function = NULL,
  verbose = TRUE,
  entity_col = "entity",
  type_col = "entity_type"
)
```

vec_preprocess 51

Arguments

Value

A data frame of filtered entities

vec_preprocess

Vectorized preprocessing of text

Description

This function preprocesses text data using vectorized operations for better performance.

This function preprocesses text data using vectorized operations for better performance.

```
vec_preprocess(
  text_data,
  text_column = "abstract",
  remove_stopwords = TRUE,
  custom_stopwords = NULL,
 min_word_length = 3,
 max_word_length = 50,
  chunk\_size = 100
)
vec_preprocess(
  text_data,
  text_column = "abstract",
  remove_stopwords = TRUE,
  custom_stopwords = NULL,
  min_word_length = 3,
 max_word_length = 50,
  chunk_size = 100
)
```

52 visualize_abc_network

Arguments

```
text_data A data frame containing text data.

text_column Name of the column containing text to process.

remove_stopwords

Logical. If TRUE, removes stopwords.

custom_stopwords

Character vector of additional stopwords to remove.

min_word_length

Minimum word length to keep.

max_word_length

Maximum word length to keep.

chunk_size

Number of documents to process in each chunk.
```

Value

A data frame with processed text.

A data frame with processed text.

Description

Create a network visualization of ABC connections using base R graphics.

Usage

```
vis_abc_network(
  abc_results,
  top_n = 25,
  min_score = 0.1,
  node_size_factor = 3,
  edge_width_factor = 1,
  color_by = "type",
  title = "ABC Model Network"
)
```

Arguments

```
abc_results A data frame containing ABC results from apply_abc_model().

top_n Number of top results to visualize.

min_score Minimum score threshold for including connections.

node_size_factor
Factor for scaling node sizes.
```

vis_abc_heatmap 53

```
edge_width_factor
```

Factor for scaling edge widths.

color_by Column to use for node colors. Default is 'type'.

title Plot title.

Value

NULL invisibly. The function creates a plot as a side effect.

vis_abc_heatmap

Create a heatmap of ABC connections

Description

This function creates a heatmap visualization of ABC connections using base R graphics.

Usage

```
vis_abc_heatmap(
  abc_results,
  top_n = 25,
  min_score = 0.1,
  show_labels = TRUE,
  title = "ABC Connections Heatmap"
)
```

Arguments

 $abc_results \qquad A \ data \ frame \ containing \ ABC \ results \ from \ apply_abc_model().$

top_n Number of top results to visualize.

min_score Minimum score threshold for including connections.

show_labels Logical. If TRUE, shows labels on the tiles.

title Plot title.

Value

NULL invisibly. The function creates a plot as a side effect.

vis_heatmap

vis_heatmap

Create an enhanced heatmap of ABC connections

Description

This function creates an improved heatmap visualization of ABC connections that can display entity type information when available, without enforcing type constraints.

Usage

```
vis_heatmap(
  abc_results,
  top_n = 25,
  min_score = 0.1,
  show_significance = TRUE,
  color_palette = "blues",
  title = "ABC Connections Heatmap",
  show_entity_types = TRUE
)
```

Arguments

Value

NULL invisibly. The function creates a plot as a side effect.

vis_network 55

vis_network

Create an enhanced network visualization of ABC connections

Description

This function creates an improved network visualization of ABC connections that displays entity types when available, without enforcing type constraints.

Usage

```
vis_network(
  abc_results,
  top_n = 25,
  min_score = 0.1,
  show_significance = TRUE,
  node_size_factor = 5,
  color_by = "type",
  title = "ABC Model Network",
  show_entity_types = TRUE,
  label_size = 1,
  layout_seed = NULL
)
```

Arguments

```
A data frame containing ABC results.
abc_results
                  Number of top results to visualize.
top_n
                  Minimum score threshold for including connections.
min_score
show_significance
                  Logical. If TRUE, highlights significant connections.
node_size_factor
                  Factor for scaling node sizes.
color_by
                  Column to use for node colors. Default is 'type'.
title
                  Plot title.
show_entity_types
                  Logical. If TRUE, includes entity types in node labels.
                  Relative size for labels. Default is 1.
label_size
                  Optional seed for layout reproducibility. If NULL, no seed is set.
layout_seed
```

Value

NULL invisibly. The function creates a plot as a side effect.

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