Package 'MIC'

June 5, 2025

```
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Version 1.1.0
Description Analyse, plot, and tabulate antimicrobial minimum inhibitory concentration (MIC) data.
     Validate the results of an MIC experiment by comparing observed MIC values to
     a gold standard assay, in line with standards from the International Organization for
     Standardization (2021) <a href="https:">https:</a>
     //www.iso.org/standard/79377.html>. Perform MIC prediction from
     whole genome sequence data stored in the Pathosystems Resource Integration Center (2013)
     <doi:10.1093/nar/gkt1099> database or locally.
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```

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as.sir_vectorised

Convert MIC or Disk Diffusion to SIR, vectorised over antimicrobials

Description

The AMR::as.sir function is not vectorised over antimicrobials. This function provides vectorisation over antimicrobials. Due to the overhead of running AMR::as.sir, this function tries to be efficient by only running AMR::as.sir as little as necessary.

Usage

```
as.sir_vectorised(mic, mo, ab, accept_ecoff = FALSE, ...)
```

Arguments

mic	vector of MIC values
mo	vector of microorganism names
ab	vector of antibiotic names
accept_ecoff	if TRUE, ECOFFs will be used when no clinical breakpoints are available
• • •	additional arguments that are passed to AMR::as.sir

Value

S3 sir values

```
\label{eq:mic} \begin{array}{llll} \mbox{mic} <-c \, ("<0.25", "8", "64", ">64") \\ \mbox{mo} <-c \, ("B_{ESCHR_{COLI"}}, "B_{ESCHR_{COLI"}}, "B_{ESCHR_{COLI"}}, "B_{ESCHR_{COLI"}}) \\ \mbox{ab} <-c \, ("AMK", "AMK", "AMK", "AMK") \\ \mbox{as.sir_vectorised(mic, mo, ab)} \\ \mbox{\# using different microorganisms and antibiotics} \\ \mbox{mic} <-c \, ("<0.25", "8", "64", ">64") \\ \mbox{mo} <-c \, ("B_{ESCHR_{COLI"}}, "B_{ESCHR_{COLI"}}, "B_{PROTS_{MRBL"}}, "B_{PROTS_{MRBL"}}) \\ \mbox{ab} <-c \, ("AMK", "AMK", "CIP", "CIP") \\ \mbox{as.sir_vectorised(mic, mo, ab)} \end{array}
```

dean_raw_mic

bias

Calculate MIC bias

Description

Calculate the bias between two AMR::mic vectors. The bias is calculated as the percentage of test MICs that are above the gold standard MICs minus the percentage of test MICs that are below the gold standard MICs.

Usage

```
bias(gold_standard, test)
```

Arguments

gold_standard AMR::mic vector test AMR::mic vector

Value

numeric value

References

International Organization for Standardization. ISO 20776-2:2021 Available from: https://www.iso.org/standard/79377.html

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
bias(gold_standard, test)</pre>
```

clean_raw_mic

Clean up raw MIC for use as a feature

Description

Removes leading "=" which can sometimes be present in raw MIC results. Also converts cotrimoxazole to trimethprim component only.

Usage

```
clean_raw_mic(mic)
```

Arguments

mic

character containing MIC/s

combined_file_system 5

Value

character of clean MIC/s

Examples

```
clean_raw_mic(c("==>64","0.25/8.0"))
```

combined_file_system Combine train and test filesystem into single folder

Description

This function reorganises files that have been split into train and test directories using train_test_filesystem() back into a single directory. This is a convenience function to reverse the effects of train_test_filesystem().

Usage

```
combined_file_system(
  path_to_folders,
  file_ext,
  train_folder = "train",
  test_folder = "test",
  overwrite = FALSE
)
```

Arguments

```
path_to_folders

path containing test and train folders; files will be moved here
file_ext file extension to filter

train_folder train folder subdirectory name

test_folder test folder subdirectory name

overwrite force overwrite of files that already exist
```

Value

Logical vector, indicated success or failure for each file

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()
# remove any existing .fna files
file.remove(
  list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)</pre>
```

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compare_mic

Compare and validate MIC values

Description

This function compares an vector of MIC values to another. Generally, this is in the context of a validation experiment – an investigational assay or method (the "test") is compared to a gold standard. The rules used by this function are in line with "ISO 20776-2:2021 Part 2: Evaluation of performance of antimicrobial susceptibility test devices against reference broth micro-dilution."

There are two levels of detail that are provided. If only the MIC values are provided, the function will look for essential agreement between the two sets of MIC. If the organism and antibiotic arguments are provided, the function will also calculate the categorical agreement using EUCAST breakpoints (or, if breakpoint not available and accept_ecoff = TRUE, ECOFFs).

The function returns a special dataframe of results, which is also an mic_validation object. This object can be summarised using summary() for summary metrics, plotted using plot() for an essential agreement confusion matrix, and tabulated using table().

Usage

```
compare_mic(
  gold_standard,
  test,
  ab = NULL,
  mo = NULL,
  accept_ecoff = FALSE,
  simplify = TRUE,
  ea_mode = "categorical",
  tolerate_censoring = "gold_standard",
  tolerate_matched_censoring = "both",
  ...
)
```

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Arguments

gold_standard vector of MICs to compare against.

test vector of MICs that are under investigation

ab character vector (same length as MIC) of antibiotic names (optional)

mo character vector (same length as MIC) of microorganism names (optional)

accept_ecoff if TRUE, ECOFFs will be used when no clinical breakpoints are available

simplify if TRUE, MIC values will be coerced into the closest halving dilution (e.g., 0.55

will be converted to 0.5)

ea_mode "categorical" or "numeric", see essential_agreement

tolerate_censoring

"strict", "gold_standard", "test", or "both" - how to handle censored data (see essential_agreement for details). Generally, this should be left as "gold_standard" since this setting "tolerates" a test that has higher granularity (i.e., less censoring) than the gold standard. Setting to "test" or "both" should be used with caution but may be appropriate in some cases where the test also produces censored results.

tolerate_matched_censoring

"strict", "gold_standard", "test", or "both" - how to handle situations where one of the values is censored, but both values match (e.g., gold_standard = ">2", test = "2"). Generally, this should be left as "both", since these values are considered to be in essential agreement. For more details, see essential_agreement.

... additional arguments to be passed to AMR::as.sir

Value

S3 mic_validation object

```
# Just using MIC values only
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
summary(val)

# Using MIC values and antibiotic and organism names
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
ab <- c("AMK", "AMK", "AMK", "AMK")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI")
val <- compare_mic(gold_standard, test, ab, mo)
"error" %in% names(val) # val now has categorical agreement</pre>
```

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compare_sir

Compare SIR results and generate categorical agreement

Description

Compare two AMR::sir vectors and generate a categorical agreement vector with the following levels: M (major error), vM (very major error), m (minor error). The error definitions are:

- 1. Major error (M): The test result is resistant (R) when the gold standard is susceptible (S).
- 2. vM (very major error): The test result is susceptible (S) when the gold standard is resistant (R).
- 3. Minor error (m): The test result is intermediate (I) when the gold standard is susceptible (S) or resistant (R), or vice versa.

Usage

```
compare_sir(gold_standard, test)
```

Arguments

```
gold_standard Susceptibility results in AMR::sir format test Susceptibility results in AMR::sir format
```

Value

factor vector with the following levels: M, vM, m.

Examples

```
gold_standard <- c("S", "R", "I", "I")
gold_standard <- AMR::as.sir(gold_standard)
test <- c("S", "I", "R", "R")
test <- AMR::as.sir(test)
compare_sir(gold_standard, test)</pre>
```

 ${\tt download_patric_db}$

Download PATRIC database

Description

Download PATRIC database

Usage

```
download_patric_db(save_path, ftp_path = patric_ftp_path, overwrite = FALSE)
```

Arguments

save_path Save path (should be .txt)

ftp_path PATRIC database FTP path to download

overwrite Force overwrite

Value

TRUE if successful, FALSE if failure.

Examples

```
download_patric_db(tempfile())
```

droplevels.mic_validation

Droplevels for MIC validation object

Description

Quite often, MIC values are being compared across methods with different levels of granularity. For example, the true MIC may be measured across a higher range of values than the test method. This means that there may be MIC levels that don't provide much additional information (since they are only present in one of the methods). This function removes these unnecessary levels at both ranges of the MIC values.

This function ensure that the changes do not "change" the essential agreement interpretation. This can be suppressed using safe = FALSE, however this is probably not desired behaviour.

Usage

```
## S3 method for class 'mic_validation'
droplevels(x, safe = TRUE, ...)
```

Arguments

x mic_validation object

safe ensure that essential agreement is not changed after dropping levels

... additional arguments

Value

mic_validation object

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Examples

```
gold_standard <- c("<0.25", "0.25", "0.5", "1", "2", "1", "0.5")
test <- c("0.004", "0.08", "<0.25", "0.5", "1", "0.5", "0.5")
val <- compare_mic(gold_standard, test)
droplevels(val)</pre>
```

ecoffs

ECOFF data

Description

A dataset containing the epidemiological cut-off values (ECOFFs) for different antibiotics and microorganisms. Currently, only the ECOFF values for *Escherichia coli* are included.

Usage

ecoffs

Format

ecoffs:

A data frame with 85 rows and 25 columns:

organism Microorganism code in AMR::mo format

antibiotic Antibiotic code in AMR::ab format

0.002:512 Counts of isolates in each concentration "bin"

Distributions see EUCAST documentation below

Observations Number of observations

(T)ECOFF see EUCAST documentation below

Confidence interval see EUCAST documentation below

Source

```
EUCAST https://www.eucast.org/mic_and_zone_distributions_and_ecoffs
```

These data have (or this document, presentation or video has) been produced in part under ECDC service contracts and made available by EUCAST at no cost to the user and can be accessed on the EUCAST website www.eucast.org. The views and opinions expressed are those of EUCAST at a given point in time. EUCAST recommendations are frequently updated and the latest versions are available at www.eucast.org.

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essential_agreement

Essential agreement for MIC validation

Description

Essential agreement calculation for comparing two MIC vectors.

Usage

```
essential_agreement(
   x,
   y,
   coerce_mic = TRUE,
   tolerate_censoring = "strict",
   tolerate_matched_censoring = "both",
   mode = "categorical"
)
```

Arguments

```
x AMR::mic or coercible y AMR::mic or coercible coerce_mic convert to AMR::mic tolerate_censoring  
    "strict", "x", "y", or "both" - whether to tolerate censoring in x, y, or both. See details.  

tolerate_matched_censoring  
    "strict", "x", "y", or "both" - how to handle situations where one of the values is censored, but both values match (e.g., x = ">2", y = "2"). For most situations, this is considered essential agreement. so should be left as "both".  

mode  
"categorical" or "numeric", see details
```

Details

Essential agreement is a central concept in the comparison of two sets of MIC values. It is most often used when validating a new method against a gold standard. This function reliably performs essential agreement in line with ISO 20776-2:2021. The function can be used in two modes: categorical and numeric. In categorical mode, the function will use traditional MIC concentrations to determine the MIC (therefore it will use force_mic() to convert both x and y to a clean MIC – see force_mic). In numeric mode, the function will compare the ratio of the two MICs, after removing censoring (values that are ">" and "<" are multiplied and divided by 2, respectively — see mic_uncensor). In most cases, categorical mode provides more reliable results. Values within +/- 1 dilutions are considered to be in essential agreement.

The tolerate_censoring argument controls how the function handles censored data. If set to "strict", the function will return NA for any pair of values that are both censored (and not equal). If set to "x" or "y", the function will allow one of the values to be censored and will compare the uncensored

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value to the other value. When set to "both", the function will allow one of the values to be censored. If using "both" and both values are censored, the function will attempt to determine essential agreement based on the ratio of the two values, but a warning will be raised.

Value

logical vector

References

International Organization for Standardization. ISO 20776-2:2021 Available from: https://www.iso.org/standard/79377.html

Examples

```
x <- AMR::as.mic(c("<0.25", "8", "64", ">64"))
y <- AMR::as.mic(c("<0.25", "2", "16", "64"))
essential_agreement(x, y)
# TRUE FALSE FALSE TRUE

# examples using tolerate_censoring
x <- AMR::as.mic("<4")
y <- AMR::as.mic("0.25")

essential_agreement(x, y, tolerate_censoring = "x") # TRUE
essential_agreement(x, y, tolerate_censoring = "y") # FALSE
essential_agreement(x, y, tolerate_censoring = "both") # TRUE (same as "x")
# strict returns FALSE as it wants the censoring cut-offs to be close
essential_agreement(x, y, tolerate_censoring = "strict")</pre>
```

example_mics

Example MIC data

Description

Example minimum inhibitory concentration validation data for three antimicrobials on Escherichia coli strains. This data is synthetic and generated to give an example of different MIC distribution.

Usage

```
example_mics
```

Format

```
example_mics:
A data frame with 300 rows and 4 columns:
gs Gold standard MICs
test Test MICs
mo Microorganism code in AMR::mo format
ab Antibiotic code in AMR::ab format
```

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Source

Synthetic data

```
fill_dilution_levels Fill MIC dilution levels
```

Description

Fill MIC dilution levels

Usage

```
fill_dilution_levels(x, cap_upper = TRUE, cap_lower = TRUE, as.mic = TRUE)
```

Arguments

X	MIC vector
cap_upper	If True, will the top level will be the highest MIC dilution in x
cap_lower	If True, will the bottom level will be the lowest MIC dilution in x
as.mic	By default, returns an ordered factor. Set as.mic = TRUE to return as AMR::mic

Value

```
ordered factor (or AMR::mic if as.mic = TRUE)
```

Examples

```
# use in combination with droplevels to clean up levels: x <- AMR::as.mic(c("<0.25", "8", "64", ">64")) x <- droplevels(x) fill_dilution_levels(x)
```

force_mic

Force MIC-like into MIC-compatible format

Description

Convert a value that is "almost" an MIC into a valid MIC value.

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Usage

```
force_mic(
  value,
  levels_from_AMR = FALSE,
  max_conc = 512,
  min_conc = 0.002,
  method = "closest",
  prefer = "max"
)
```

Arguments

value vector of MIC-like values (numeric or character)

levels_from_AMR

conform to AMR::as.mic levels

max_conc maximum concentration to force to min_conc minimum concentration to force to

method method to use when forcing MICs (closest or round_up)

prefer where value is in between MIC (e.g., 24mg/L) chose the higher MIC ("max") or

lower MIC ("min"); only applies to method = "closest"

Details

Some experimental or analytical conditions measure MIC (or surrogate) in a way that does not fully conform to traditional MIC levels (i.e., concentrations). This function allows these values to be coerced into an MIC value that is compatible with the AMR::mic class. When using method = "closest", the function will choose the closest MIC value to the input value (e.g., 2.45 will be coerced to 2). When using method = "round up", the function will round up to the next highest MIC value (e.g., 2.45 will be coerced to 4). "Round up" is technically the correct approach if the input value was generated from an experiment that censored between concentrations (e.g., broth or agar dilution). However, "closest" may be more appropriate in some cases.

Value

AMR::as.mic compatible character

```
force_mic(c("2.32", "<4.12", ">1.01"))
```

```
genomes_to_kmer_libsvm
```

Convert genomes to kmers in libsym format

Description

Raw genome data (pre- or post-assembly) is usually transformed by k-mer counting prior to machine learning (ML). XGBoost is a popular ML algorithm for this problem, due to its scalability to high dimensional data. This function converts genomes to k-mer counts stored in XGBoost's preferred format, libsvm. Further information on the libsvm format is available at https://xgboost.readthedocs.io/en/stable/tutorials/input_format.html. Briefly, libsvm is effectively a text file that stores data points as x:y pairs, where x is the feature index, and y is the feature value. Each observation is stored on its own line, with the first column reserved for labels. Labels can be provided later, during data import.

This function converts each individual genome to an individual libsvm text file of k-mer counts (therefore, each .txt file will be 1 line long). This function supports parallel processing using the by setting an appropriate future::plan() (usually future::multisession) — each genome is processed in parallel. To monitor progress, use the progressr package by wrapping the function in with_progress.

Although XGBoost can load a multiple .txt (libsvm) files by providing the directory as an input, this is generally not recommended as order of import cannot be guaranteed and probably depends on filesystem. Instead, it is recommended that this function is combined with split_and_combine_files() which generates a single .txt file (with the order of observations guaranteed and stored in a .csv file).

Usage

```
genomes_to_kmer_libsvm(
  source_dir,
  target_dir,
  k = 3,
  canonical = TRUE,
  squeeze = FALSE,
  ext = ".fna"
)
```

Arguments

```
source_dir directory containing genomes

target_dir target directory to store kmers in libsvm format

k k-mer length

canonical only count canonical kmers

squeeze remove non-canonical kmers

ext file extension to filter
```

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Value

TRUE if successful

See Also

to convert a single genome, use genome_to_libsvm()

Examples

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()</pre>
# remove any existing .fna files
file.remove(
list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
for (i in 1:10) {
100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
tmp_target_dir <- file.path(tmp_dir, "kmers")</pre>
unlink(tmp_target_dir, recursive = TRUE)
# convert genomes to k-mers
future::plan(future::sequential) # use multisession for parallel processing
progressr::with_progress(
 genomes_to_kmer_libsvm(tmp_dir, tmp_target_dir, k = 3)
# check the output
list.files(tmp_target_dir)
readLines(list.files(tmp_target_dir, full.names = TRUE)[1])
```

genome_to_libsvm

Converts a genome to kmers stored in libsym format on disk

Description

This function converts a single genome to a libsym file containing kmer counts. The libsym format will be as follows:

```
label 1:count 2:count 3:count ...
```

Label is optional and defaults to 0. The kmer counts are indexed by the kmer index, which is the lexicographically sorted index of the kmer. Libsvm is a sparse format.

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Usage

```
genome_to_libsvm(
    x,
    target_path,
    label = as.character(c("0")),
    k = 3L,
    canonical = TRUE,
    squeeze = FALSE,
    overwrite = FALSE
)
```

Arguments

x genome in string format

target_path path to store libsvm file (.txt)

label libsym label k kmer length

canonical only record canonical kmers (i.e., the lexicographically smaller of a kmer and

its reverse complement)

squeeze remove non-canonical kmers

overwrite overwrite existing file

Value

boolean indicating success

See Also

For multiple genomes in a directory, processed in parallel, see genomes_to_kmer_libsvm()

For more details on libsvm format, see https://xgboost.readthedocs.io/en/stable/tutorials/input_format.html

```
temp_libsvm_path <- tempfile(fileext = ".txt")
genome_to_libsvm("ATCGCAGT", temp_libsvm_path)
readLines(temp_libsvm_path)</pre>
```

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get_mic

Get MIC meta-data from feature database

Description

This function helps extract MICs from a database of results. It is compatible with the PATRIC meta data format when used on a tidy_patric_db object, created using tidy_patric_db().

If more than one MIC is present for a particular observation, the function can return the higher MIC by setting prefer_high_mic = TRUE. If prefer_high_mic = FALSE, the lower MIC will be returned.

Usage

```
get_mic(
  х,
  ids,
  ab_col,
  id_col = NULL,
  as_mic = TRUE,
 prefer_high_mic = TRUE,
  simplify = TRUE
)
```

Arguments

```
Х
                  dataframe containing meta-data
                  vector of IDs to get meta-data for
ids
ab_col
                  column name containing MIC results
id_col
                  column name containing IDs
as_mic
                  return as AMR::as.mic
prefer_high_mic
                  where multiple MIC results per ID, prefer the higher MIC
                 return as vector of MICs (vs dataframe)
simplify
```

Value

vector containing MICs, or dataframe of IDs and MICs

```
df \leftarrow data.frame(genome_id = c("a_12", "b_42", "x_21", "x_21", "r_75"),
                  gentamicin = c(0.25, 0.125, 32.0, 16.0, "<0.0125"))
get_mic(df,
        ids = c("b_42", "x_21"),
        ab_col = "gentamicin",
        id_col = "genome_id",
        as_mic = FALSE,
```

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```
prefer_high_mic = TRUE,
simplify = TRUE)
```

kmers

Generates genome kmers

Description

Generates genome kmers

Usage

```
kmers(
    x,
    k = 3L,
    simplify = FALSE,
    canonical = TRUE,
    squeeze = FALSE,
    anchor = TRUE,
    clean_up = TRUE,
    key_as_int = FALSE,
    starting_index = 1L
)
```

Arguments

X	genome in string format
k	kmer length
simplify	returns a numeric vector of kmer counts, without associated string. This is useful to save memory, but should always be used with anchor = true.
canonical	only record canonical kmers (i.e., the lexicographically smaller of a kmer and its reverse complement)
squeeze	remove non-canonical kmers
anchor	includes unobserved kmers (with counts of 0). This is useful when generating a dense matrix where kmers of different genomes align.
clean_up	only include valid bases (ACTG) in kmer counts (excludes non-coding results such as N)
key_as_int	return kmer index (as "kmer_index") rather than the full kmer string. Useful for index-coded data structures such as libsvm.
starting_index	the starting index, only used if key_as_int = TRUE.

Value

list of kmer values, either as a list of a single vector (if simplify = TRUE), or as a named list containing "kmer_string" and "kmer_value".

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Examples

```
kmers("ATCGCAGT")
```

load_patric_db

Load PATRIC database

Description

Load PATRIC database

Usage

```
load_patric_db(x = patric_ftp_path)
```

Arguments

.,

Character path to local or ftp path (.txt or .rds), or data.frame object.

Value

```
PATRIC database (S3 class 'patric_db')
```

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mic_censor

Censor MIC values

Description

MIC datasets often arise from different laboratories or experimental conditions. In practice, this means that there can be different levels of censoring (<= and >) within the data. This function can be used to harmonise the dataset to a single level of censoring. The function requires a set of rules that specify the censoring levels (see example).

Usage

```
mic_censor(mic, ab = NULL, mo = NULL, rules = NULL, max = Inf, min = -Inf)
```

Arguments

mic		MIC (coercible to AMR::as.mic)
ab		antibiotic name (coercible to AMR::as.ab)
mo		microorganism name (coercible to AMR::as.mo)
rule	es	censor rules - named list of pathogen (in AMR::as.mo code) to antibiotic (in AMR::as.ab code) to censoring rules. The censoring rules should provide a min or max value to censor MICs to. See example for more.
max		maximum concentration to censor to (default = Inf), will override any rules provided
min		minimum concentration to censor to (default = -Inf), will override any rules provided

Value

censored MIC values (S3 mic class)

```
example_rules <- list("B_ESCHR_COLI" = list(
    "AMK" = list(min = 2, max = 32),
    "CHL" = list(min = 4, max = 64),
    "GEN" = list(min = 1, max = 16),
    "CIP" = list(min = 0.015, max = 4),
    "MEM" = list(min = 0.016, max = 16),
    "AMX" = list(min = 2, max = 64),
    "AMC" = list(min = 2, max = 64),
    "FEP" = list(min = 0.5, max = 64),
    "CAZ" = list(min = 1, max = 128),
    "TGC" = list(min = 0.25, max = 1)
    ))

mic_censor(AMR::as.mic(512),</pre>
```

22 mic_r_breakpoint

```
"AMK",
"B_ESCHR_COLI",
example_rules) == AMR::as.mic(">32")
```

mic_range

Generate dilution series

Description

Generate dilution series

Usage

```
mic_range(start = 512, dilutions = Inf, min = 0.002, precise = FALSE)
```

Arguments

start starting (highest) concentration

dilutions number of dilutions

min minimum (lowest) concentration

precise force range to be high precision (not usually desired behaviour)

Value

Vector of numeric concentrations

Examples

```
mic_range(128)
mic_range(128, dilutions = 21) # same results
```

mic_r_breakpoint

R breakpoint for MIC

Description

R breakpoint for MIC

Usage

```
mic_r_breakpoint(mo, ab, accept_ecoff = FALSE, ...)
```

mic_s_breakpoint 23

Arguments

mo mo name (coerced using AMR::as.mo)
ab ab name (coerced using AMR::as.ab)

accept_ecoff if TRUE, ECOFFs will be used when no clinical breakpoints are available

additional arguments to pass to AMR::as.sir, which is used to calculate the R

breakpoint

Value

MIC value

Examples

```
mic_r_breakpoint("B_ESCHR_COLI", "AMK")
mic_r_breakpoint("B_ESCHR_COLI", "CHL", accept_ecoff = TRUE)
```

mic_s_breakpoint

S breakpoint for MIC

Description

S breakpoint for MIC

Usage

```
mic_s_breakpoint(mo, ab, accept_ecoff = FALSE, ...)
```

Arguments

mo mo name (coerced using AMR::as.mo)
ab ab name (coerced using AMR::as.ab)

accept_ecoff if TRUE, ECOFFs will be used when no clinical breakpoints are available

... additional arguments to pass to AMR::as.sir, which is used to calculate the S

breakpoint

Value

MIC value

```
mic_s_breakpoint("B_ESCHR_COLI", "AMK")
mic_s_breakpoint("B_ESCHR_COLI", "CHL", accept_ecoff = TRUE)
```

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mic_uncensor

Uncensor MICs

Description

Uncensor MICs

Usage

```
mic_uncensor(
  mic,
  method = "scale",
  scale = 2,
  ab = NULL,
  mo = NULL,
  distros = NULL
)
```

Arguments

mic vector of MICs to uncensor; will be coerced to MIC using AMR::as.mic
method method to uncensor MICs (scale, simple, or bootstrap)
scale scalar to multiply or divide MIC by (for method = scale)
ab antibiotic name (for method = bootstrap)
mo microorganism name (for method = bootstrap)
distros dataframe of epidemiological distributions (only used, optionally, for method = bootstrap)

Details

Censored MIC data is generally unsuitable for modelling without some conversion of censored data. The default behaviour (method = scale) is to halve MICs under the limit of detection (<=) and double MICs above the limit of detection (>). When used with method = simple, this function effectively just removes the censoring symbols, e.g., <=2 becomes 2, and >64 becomes 64.

The bootstrap method is the more complex of the three available methods. It attempts to use a second (uncensored) MIC distribution to sample values in the censored range. These values are then used to populate and uncensor the MIC data provided as input (mic). The second (uncensored) MIC distribution is ideally provided from similar experimental conditions. Alternatively, epidemiological distributions can be used. These distributions should be provided as a dataframe to the distros argument. The format for this dataframe is inspired by the EUCAST epidemiological distributions, see: https://www.eucast.org/mic_and_zone_distributions_and_ecoffs. The dataframe should contain columns for antimicrobial (converted using AMR::as.ab), organism (converted using AMR::as.mo), and MIC concentrations. An example is provided in the 'ecoffs' dataset available with this pacakge. Currently, only Escherichia coli is available in this dataset. Each observation (row) consists of the frequency a particular MIC concentration is observed in the distribution. If such a dataframe is not provided to distros, the function will attempt to use 'ecoffs', but remains limited to E. coli.

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Value

vector of MICs in AMR::mic format

References

https://www.eucast.org/mic_and_zone_distributions_and_ecoffs

Examples

```
mic_uncensor(c(">64.0", "<0.25", "8.0"), method = "scale", scale = 2)
```

move_files

Move or copy files using logical vector

Description

This is simply a wrapper around file.copy/file.rename that allows for filtering by a logical vector (move_which). This can replicate the behaviour of a predicate function (see example), and may be easier to read.

Usage

```
move_files(source_dir, target_dir, move_which, ext = ".txt", copy = FALSE)
```

Arguments

```
source_dir move from directory
target_dir move to directory
move_which logical vector to filter (or use TRUE to move all)
ext file extension to filter
copy copy files (rather than move)
```

Value

Logical vector, indicating success or failure for each file

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()
# remove any existing .fna files
file.remove(
  list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)
for (i in 1:10) {
  writeLines(paste0(">", i, "\n", paste0(sample(c("A", "T", "C", "G"),
```

26 plot.mic_validation

plot.mic_validation

Plot MIC validation results

Description

Plot MIC validation results

Usage

```
## $3 method for class 'mic_validation'
plot(
    x,
    match_axes = TRUE,
    add_missing_dilutions = TRUE,
    facet_wrap_ncol = NULL,
    facet_wrap_nrow = NULL,
    ...
)
```

Arguments

x object generated using compare_mic

match_axes Same x and y axis

add_missing_dilutions

Axes will include dilutions that are not

facet_wrap_ncol

Facet wrap into n columns by antimicrobial (optional, only available when more than one antimicrobial in validation)

facet_wrap_nrow

Facet wrap into n rows by antimicrobial (optional, only available when more than one antimicrobial in validation) represented in the data, based on a series of dilutions generated using mic_range().

.. additional arguments

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Value

ggplot object

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
plot(val)

# if the validation contains multiple antibiotics, i.e.,
ab <- c("CIP", "CIP", "AMK", "AMK")
val <- compare_mic(gold_standard, test, ab)
# the following will plot all antibiotics in a single plot (pooled results)
plot(val)
# use the faceting arguments to split the plot by antibiotic
plot(val, facet_wrap_ncol = 2)</pre>
```

print.mic_validation Print MIC validation object

Description

Print MIC validation object

Usage

```
## S3 method for class 'mic_validation'
print(x, ...)
```

Arguments

```
x mic_validation object
... additional arguments
```

Value

character

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
print(val)</pre>
```

Description

Print MIC validation summary

Usage

```
## S3 method for class 'mic_validation_summary' print(x, ...)
```

Arguments

```
x mic_validation_summary object
... additional arguments
```

Value

character

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
print(summary(val))</pre>
```

pull_PATRIC_genomes

Automated download of genomes from PATRIC database

Description

Automated download of genomes from PATRIC database

Usage

```
pull_PATRIC_genomes(
  output_directory,
  taxonomic_name = NULL,
  database = patric_ftp_path,
  filter = "MIC",
  ab = NULL,
  n_genomes = 0
)
```

qc_in_range 29

Arguments

```
output_directory
local directory to save to

taxonomic_name character of taxonomic bacterial name to download

database local or ftp path to PATRIC database, or loaded database using load_patric_db()

filter "MIC" or "disk" or "all" phenotypes

ab antibiotic(s) of interest, provided as a character vector of antibiotic names/codes, or ideally, as AMR::ab classes, created using AMR::as.ab (default = all)

n_genomes number of genomes (0 = all)
```

Value

The number of failed downloads (i.e., 0 if all attempted downloads were successful).

Examples

qc_in_range

Check that MIC is within QC range

Description

Check whether MIC values are within acceptable range for quality control (QC). Every MIC experiment should include a control strain with a known MIC. The results of the experiment are only valid if the control strain MIC falls within the acceptable range. This function checks whether an MIC result is within the acceptable range given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI). The acceptable range is defined by 'QC_table', which is a dataset which is loaded with this package.

The source of the QC values is the WHONET QC Ranges and Targets available from the 'Antimicrobial Resistance Test Interpretation Engine' (AMRIE) repository: https://github.com/AClark-WHONET/AMRIE

Usage

```
qc_in_range(
  measurement,
  strain,
  ab,
  ignore_na = TRUE,
  guideline = "EUCAST",
  year = "2023"
)
```

30 qc_on_target

Arguments

measurement measured QC MIC

strain control strain identifier (usually ATCC)

ab antibiotic name (will be coerced to AMR::as.ab)

ignore_na ignores NA (returns TRUE)

guideline Guideline to use (EUCAST or CLSI)

year Guideline year (version)

Value

logical vector

References

O'Brien TF, Stelling JM. WHONET: An Information System for Monitoring Antimicrobial Resistance. Emerg Infect Dis. 1995 Jun;1(2):66–66.

Examples

```
qc_in_range(AMR::as.mic(0.5), 25922, "GEN") == TRUE
qc_in_range(AMR::as.mic(8.0), 25922, "GEN") == FALSE
```

qc_on_target

Check that QC measurement is at the required target [Experimental]

Description

MIC experiments should include a control strain with a known MIC. The MIC result for the control strain should be a particular target MIC. This function checks whether the target MIC was achieved given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI).

Since QC target values are currently not publicly available in an easy to use format, this function takes a pragmatic approach – for most antibiotics and QC strains, the target is assumed to be the midpoint of the acceptable range. This approximation is not necessarily equal to the QC target reported by guideline setting bodies such as EUCAST. Therefore, this function is considered experimental and should be used with caution.

This function can be used alongnside qc_in_range(), which checks whether the MIC is within the acceptable range.

The source of the QC values is the WHONET QC Ranges and Targets available from the 'Antimicrobial Resistance Test Interpretation Engine' (AMRIE) repository: https://github.com/AClark-WHONET/AMRIE

Usage

```
qc_on_target(
  measurement,
  strain,
  ab,
  ignore_na = TRUE,
  guideline = "EUCAST",
  year = "2023"
)
```

Arguments

measurement measured QC MIC
strain control strain identifier (usually ATCC)
ab antibiotic name (will be coerced to AMR::as.ab)
ignore_na ignores NA (returns TRUE)
guideline Guideline to use (EUCAST or CLSI)

year Guideline year (version)

Value

logical vector

References

O'Brien TF, Stelling JM. WHONET: An Information System for Monitoring Antimicrobial Resistance. Emerg Infect Dis. 1995 Jun;1(2):66–66.

Examples

```
qc_on_target(AMR::as.mic(0.5), 25922, "GEN") == TRUE
```

```
replace_multiple_slashes
```

Removes multiple slashes in a path or url

Description

Removes multiple slashes in a path or url

Usage

```
replace_multiple_slashes(path)
```

Arguments

path character vector

Value

character vector of paths without duplicate slashes

reverse_complement

Reverse complement of DNA string

Description

Reverse complement of DNA string

Usage

```
reverse_complement(dna)
```

Arguments

dna

DNA string

Value

reverse complement of DNA string

Examples

```
reverse_complement("ATCG")
```

```
split_and_combine_files
```

Create test train files from a number of files

Description

This function combines files into a train and test set, stored on disk. It can be used in combination with genomes_to_kmer_libsvm() to create a dataset that can be loaded into XGBoost (either by first creating an xgboost::DMatrix, or by using the data argument in xgboost::xgb.train() or xg-boost::xgb.cv()). The following three files will be created:

- 1. train.txt the training data
- 2. test.txt the testing data (if split < 1)
- 3. names.csv a csv file containing the original filenames and their corresponding type (train or test)

The function will check if the data is already in the appropriate format and will not overwrite unless forced using the overwrite argument.

By providing 1.0 to the split argument, the function can be used to combine files without a train-test split. In this case, all the files will be classed as 'train', and there will be no 'test' data. This is useful if one wants to perform cross-validation using xgboost::xgb.cv() or MIC::xgb.cv.lowmem(). It is also possible to combine all data into train and then perform splitting after loading into an xgboost::DMatrix, using xgboost::slice().

Usage

```
split_and_combine_files(
  path_to_files,
  file_ext = ".txt",
  split = 0.8,
  train_target_path = NULL,
  test_target_path = NULL,
  names_backup = NULL,
  shuffle = TRUE,
  overwrite = FALSE
)
```

Arguments

```
path_to_files
                   path containing files or vector of filepaths
file_ext
                   file extension to filter
split
                   train-test split
train_target_path
                   name of train file to save as (by default, will be train.txt in the path_to_files
                   directory)
test_target_path
                   name of test file to save as (by default, will be test.txt in the path to files direc-
                   name of file to save backup of filename metadata (by default, will be names.csv
names_backup
                   in the path_to_files directory)
shuffle
                   randomise prior to splitting
overwrite
                   overwrite target files
```

Value

named list of paths to created train/test files, original filenames

```
set.seed(123)
# create 10 random libsvm files
tmp_dir <- tempdir()
# remove any existing .txt files</pre>
```

```
file.remove(
list.files(tmp_dir, pattern = "*.txt", full.names = TRUE)
for (i in 1:10) {
 # each line is K: V
 writeLines(paste0(i, ": ", paste0(sample(1:100, 10, replace = TRUE),
 collapse = " ")), file.path(tmp_dir, paste0(i, ".txt")))
 # split files into train and test directories
 paths <- split_and_combine_files(</pre>
  tmp_dir,
  file_ext = "txt",
  split = 0.8,
  train_target_path = file.path(tmp_dir, "train.txt"),
  test_target_path = file.path(tmp_dir, "test.txt"),
  names_backup = file.path(tmp_dir, "names.csv"),
  overwrite = TRUE)
 readLines(paths[["train"]])
```

squeezed_index_to_str Get str conversion of squeezed kmer using index

Description

Get str conversion of squeezed kmer using index

Usage

```
squeezed_index_to_str(x, k, starting_index = 1L)
```

Arguments

```
x integer vector of kmer indicesk kmer lengthstarting_index starting index (libsvm is usually indexed starting at 1)
```

Value

vector of squeezed kmer strings

```
squeezed_index_to_str(2, k = 3)
```

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squeezed_mers

Generates all permutations of squeezed kmers

Description

Generates all permutations of squeezed kmers

Usage

```
squeezed_mers(k = 3L)
```

Arguments

k

kmer length

Value

vector of squeezed kmers

Examples

squeezed_mers(3)

standardise_mic

Standardise MIC to control strain [Experimental]

Description

MIC experiments are generally quality-controlled by including a control strain with a known MIC. The MIC result for the control strain should be a particular target MIC, or at least within an acceptable range. This function standardises a measured MIC to the target MIC given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI). The definition of standardisation in this context is to adjust the measured MIC based on the QC MIC. This is based on the following principles and assumption:

- 1. A measured MIC is composed of two components: the true MIC and a measurement error. The measurement error is considered to be inevitable when measuring MICs, and is likely to be further composed of variability in laboratory conditions and operator interpretation.
- 2. It is assumed that the MIC of the control strain in the experiment has also been affected by this error.

The standardisation applied by this function uses the measured QC strain MIC as a reference point, and scales the rest of the MICs to this reference. In general, this means that the MICs are doubled or halved, depending on the result of the QC MIC. A worked example is provided below and illustrates the transformation that this function applies.

There is no current evidence base for this approach, therefore, this function is considered experimental and should be used with caution.

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Usage

```
standardise_mic(
   test_measurement,
   qc_measurement,
   strain,
   ab,
   prefer_upper = FALSE,
   ignore_na = TRUE,
   guideline = "EUCAST",
   year = "2023",
   force = TRUE
)
```

Arguments

test_measurement

Measured MIC to standardise

 ${\tt qc_measurement} \quad Measured \ QC \ MIC \ to \ standardise \ to$

strain control strain identifier (usually ATCC)

ab antibiotic name (will be coerced to AMR::as.ab)

prefer_upper Where the target MIC is a range, prefer the upper value in the range

year Guideline year (version)

force Force into MIC-compatible format after standardisation

Value

AMR::mic vector

subset.mic_validation 37

```
subset.mic\_validation Subset MIC validation object
```

Description

Subset MIC validation object

Usage

```
## S3 method for class 'mic_validation'
subset(x, subset, ...)
```

Arguments

```
x mic_validation objectsubset logical expression to subset by... additional arguments
```

Value

mic_validation object

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
ab <- AMR::as.ab(c("AMK", "AMK", "CIP", "CIP"))
mo <- AMR::as.mo(c("E. coli", "E. coli", "P. mirabilis", "P. mirabilis"))
val <- compare_mic(gold_standard, test, ab, mo)
subset(val, ab == AMR::as.ab("AMX"))
subset(val, mo == AMR::as.mo("E. coli"))</pre>
```

```
summary.mic_validation
```

Summary of MIC validation results

Description

Summarise the results of an MIC validation generated using compare_mic().

Usage

```
## S3 method for class 'mic_validation'
summary(object, ...)
```

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Arguments

```
object S3 mic_validation object
... further optional parameters
```

Value

S3 mic_validation_summary object

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
summary(val)
# or, for more detailed results
as.data.frame(summary(val))</pre>
```

table

Table

Description

Table

Usage

```
table(x, ...)
## Default S3 method:
table(x, ...)
## S3 method for class 'mic_validation'
table(
    x,
    format = "flextable",
    fill_dilutions = TRUE,
    bold = TRUE,
    ea_color = NULL,
    gold_standard_name = "Gold Standard",
    test_name = "Test",
    ...
)
```

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Arguments

x mic_validation S3 object
... further arguments

format simple or flextable

fill_dilutions Fill dilutions that are not present in the data in order to match the y- and x- axes

bold Bold cells where essential agreement is TRUE ea_color Background color for essential agreement cells

gold_standard_name

Name of the gold standard to display in output

test_name Name of the test to display in output

Value

table or flextable object

Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
table(val)</pre>
```

Description

Tidy PATRIC data

Usage

```
tidy_patric_meta_data(
    x,
    prefer_more_resistant = TRUE,
    as_ab = TRUE,
    filter_abx = NULL
)
```

Arguments

x PATRIC database loaded using MIC::load_patric_db

prefer_more_resistant

High MICs, narrow zones, or resistant phenotypes will be preferred where mul-

tiple reported for the same isolate

as_ab convert antibiotics to AMR::ab class (column names are antibiotic codes)

filter_abx filter antibiotics of interest, provided as a vector of antibiotics character names/codes,

or ideally, as AMR::ab classes, created using AMR::as.ab

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Value

Tidy data, with antimicrobials in wide format, column names describing methodology ("mic_", "disk_", "pheno_"). S3 class "tidy_patric_db".

Examples

train_test_filesystem Organise files into a train-test filesystem

Description

Organise files into a train-test filesystem

Usage

```
train_test_filesystem(
  path_to_files,
  file_ext,
  split = 0.8,
  train_folder = "train",
  test_folder = "test",
  shuffle = TRUE,
  overwrite = FALSE
)
```

Arguments

```
path_to_files directory containing files

file_ext file extension to filter

split training data split

train_folder name of training folder (subdirectory), will be created if does not exist

test_folder name of testing folder (subdirectory), will be created if does not exist

shuffle randomise files when splitting (if FALSE, files will be sorted by filename prior to splitting)

overwrite force overwrite of files that already exist
```

Value

named vector of train and test directories

Examples

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()</pre>
# remove any existing .fna files
file.remove(
 list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)
for (i in 1:10) {
writeLines(paste0(">", i, "\n", paste0(sample(c("A", "T", "C", "G"),
 100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
# split files into train and test directories
paths <- train_test_filesystem(tmp_dir,</pre>
                                file_ext = "fna",
                                split = 0.8,
                                shuffle = TRUE,
                                overwrite = TRUE)
list.files(paths[["train"]])
list.files(paths[["test"]])
```

unsqueezed_index_to_str

Get str conversion of unsqueezed kmer using index

Description

Get str conversion of unsqueezed kmer using index

Usage

```
unsqueezed_index_to_str(x, k, starting_index = 1L)
```

Arguments

```
x integer vector of kmer indicesk kmer lengthstarting_index starting index (libsvm is usually indexed starting at 1)
```

Value

vector of unsqueezed kmer strings

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Examples

```
unsqueezed_index_to_str(2, k = 3)
```

unsqueezed_mers

Generates all permutations of unsqueezed kmers

Description

Generates all permutations of unsqueezed kmers

Usage

```
unsqueezed_mers(k = 3L)
```

Arguments

k

kmer length

Value

vector of unsqueezed kmers

Examples

```
unsqueezed_mers(3)
```

xgb.cv.lowmem

Low memory cross-validation wrapper for XGBoost

Description

This function performs similar operations to xgboost::xgb.cv, but with the operations performed in a memory efficient manner. Unlike xgboost::xgb.cv, this version does not load all folds into memory from the start. Rather it loads each fold into memory sequentially, and trains trains each fold using xgboost::xgb.train. This allows larger datasets to be cross-validated.

The main disadvantage of this function is that it is not possible to perform early stopping based the results of all folds. The function does accept an early stopping argument, but this is applied to each fold separately. This means that different folds can (and should be expected to) train for a different number of rounds.

This function also allows for a train-test split (as opposed to multiple) folds. This is done by providing a value of less than 1 to nfold, or a list of 1 fold to folds. This is not possible with xg-boost::xgb.cv, but can be desirable if there is downstream processing that depends on an xgb.cv.synchromous object (which is the return object of both this function and xgboost::xgb.cv).

Otherwise, where possible this function tries to return the same data structure as xgboost::xgb.cv, with the exception of callbacks (not supported as a field within the return object). To save models, use the save_models argument, rather than the cb.cv.predict(save_models = TRUE) callback.

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Usage

```
xgb.cv.lowmem(
  params = list(),
  data,
  nrounds,
  nfold,
  label = NULL,
 missing = NA,
 prediction = FALSE,
 metrics = list(),
  obj = NULL,
  feval = NULL,
  stratified = TRUE,
  folds = NULL,
  train_folds = NULL,
  verbose = 1,
  print_every_n = 1L,
 early_stopping_rounds = NULL,
 maximize = NULL,
 save_models = FALSE,
)
```

Arguments

parameters for xgboost params data DMatrix or matrix nrounds number of training rounds number of folds, or if < 1 then the proportion will be used as the training split in nfold a train-test split data labels (alternatively provide with DMatrix) label handling of missing data (see xgb.cv) missing prediction return predictions metrics evaluation metrics obj custom objective function feval custom evaluation function stratified whether to use stratified folds folds custom folds train_folds custom train folds verbose verbosity level print every n iterations print_every_n early_stopping_rounds early stopping rounds (applied to each fold)

xgb.cv.lowmem

```
maximize whether to maximize the evaluation metric save_models whether to save the models additional arguments passed to xgb.train
```

Value

xgb.cv.synchronous object

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