

Package ‘MIC’

October 12, 2025

Title Analysis of Antimicrobial Minimum Inhibitory Concentration Data

Version 1.2.0

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) <<https://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](https://doi.org/10.1093/nar/gkt1099)> database or locally.

License GPL (>= 3)

Encoding UTF-8

RoxygenNote 7.3.3

Imports AMR, glue, readr, dplyr, Rcpp, data.table, Biostrings, stringr, rlang, tidyr, future.apply, progressr, lemon, ggplot2, forcats, purrr, tibble, curl

Depends R (>= 4.1.0)

LazyData true

LinkingTo Rcpp

Suggests testthat (>= 3.0.0), xgboost, flextable, caret, lifecycle, future

Config/testthat/edition 3

URL <https://github.com/agerada/MIC>

BugReports <https://github.com/agerada/MIC/issues>

NeedsCompilation yes

Author Alessandro Gerada [aut, cre, cph] (ORCID: <<https://orcid.org/0000-0002-6743-4271>>)

Maintainer Alessandro Gerada <alessandro.gerada@liverpool.ac.uk>

Repository CRAN

Date/Publication 2025-10-12 16:40:14 UTC

Contents

as.sir_vectorised	3
bias	4
clean_raw_mic	4
combined_file_system	5
compare_mic	6
compare_sir	8
download_patric_db	8
droplevels.mic_validation	9
ecoffs	10
essential_agreement	11
example_mics	12
fill_dilution_levels	13
force_mic	14
genomes_to_kmer_libsvm	15
genome_to_libsvm	17
get_mic	18
kmers	19
load_patric_db	21
mic_censor	21
mic_range	22
mic_r_breakpoint	23
mic_s_breakpoint	24
mic_uncensor	24
move_files	26
plot.mic_validation	27
print.mic_validation	28
print.mic_validation_summary	28
pull_PATRIC_genomes	29
qc_in_range	30
qc_on_target	31
replace_multiple_slashes	32
reverse_complement	33
split_and_combine_files	33
squeezed_index_to_str	35
squeezed_mers	36
standardise_mic	36
subset.mic_validation	38
summary.mic_validation	39
table	39
tidy_patric_meta_data	40
train_test_filesystem	41
unsqueezed_index_to_str	43
unsqueezed_mers	43
xgb.cv.lowmem	44

Index

47

as.sir_vectorised	<i>Convert MIC or Disk Diffusion to SIR, vectorised over antimicrobials</i>
-------------------	---

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

Examples

```
mic <- c("<0.25", "8", "64", ">64")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI")
ab <- c("AMK", "AMK", "AMK", "AMK")
as.sir_vectorised(mic, mo, ab)
# using different microorganisms and antibiotics
mic <- c("<0.25", "8", "64", ">64")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_PROTS_MRBL", "B_PROTS_MRBL")
ab <- c("AMK", "AMK", "CIP", "CIP")
as.sir_vectorised(mic, mo, ab)
```

bias	<i>Calculate MIC bias</i>
------	---------------------------

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)
```

clean_raw_mic	<i>Clean up raw MIC for use as a feature</i>
---------------	--

Description

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

Usage

```
clean_raw_mic(mic)
```

Arguments

mic	character containing MIC/s
-----	----------------------------

Value

character of clean MIC/s

Examples

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

combined_file_system	<i>Combine train and test filesystem into single folder</i>
----------------------	---

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

Examples

```
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"),
  100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
}

# split files into train and test directories
paths <- train_test_filesystem(tmp_dir,
                              file_ext = "fna",
                              split = 0.8,
                              shuffle = TRUE,
                              overwrite = TRUE)

# combine files back into a single directory
combined_file_system(tmp_dir, "fna")
list.files(tmp_dir)

```

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",
  tolerate_leq = TRUE,
  tolerate_geq = TRUE,
  ...
)

```

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 .
tolerate_leq	whether to tolerate <= in essential agreement, e.g., <=2 and 4 will be considered in essential agreement. See essential_agreement for details.
tolerate_geq	whether to tolerate >= in essential agreement, e.g., >=4 and 2 will be considered in essential agreement. See essential_agreement for details.
...	additional arguments to be passed to AMR::as.sir

Value

S3 mic_validation object

Examples

```
# 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
```

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)
```

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(fileext = ".txt"))
```

```
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

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)
```

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.

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",
  tolerate_leq = TRUE,
  tolerate_geq = TRUE,
  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".
tolerate_leq	whether to tolerate <= in essential agreement, e.g., <=2 and 4 will be considered in essential agreement (because <=2 includes 2mg/L, which is within 1 dilution of 4mg/L). This argument respects the tolerate_censoring argument, so if tolerate_censoring is "strict", this will not be applied.
tolerate_geq	whether to tolerate >= in essential agreement, e.g., >=4 and 2 will be considered in essential agreement (because >=4 includes 4mg/L, which is within 1 dilution of 2mg/L). This argument respects the tolerate_censoring argument, so if tolerate_censoring is strict, this will not be applied.
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 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")
```

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

Source

Synthetic data

fill_dilution_levels	<i>Fill MIC dilution levels</i>
----------------------	---------------------------------

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.

Usage

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

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"
leq	whether to force <= for lower censored values (i.e., <). If TRUE, then all values below the limit of detection are converted to <=. If FALSE, then they are converted to <. If NULL, they are not changed.
geq	whether to force >= for higher censored values (i.e., >). If TRUE, then all values above the limit of detection are converted to >=. If FALSE, then they are converted to >. If NULL, they are not changed.

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.

Please note that this function will not make any changes to censored values (beyond some simple cleaning, e.g., `<==2` is converted to `<=2`). This is because it is not possible to make assumptions about censored data.

The `leq` and `geq` arguments convert censored values to `<=` or `>=`. When MIC is measured using an inhibitory dilution method, the lower limit should be reported as `<=` (since the lowest dilution could be inhibitory itself), and the upper limit should be reported as `>` (growth in the highest dilution means that it is not an inhibitory concentration). The default values for `leq` and `geq` enforce this.

Value

`AMR::as.mic` compatible character

Examples

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

genomes_to_kmer_libsvm

Convert genomes to kmers in libsvm 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

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()  
# 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"))  
}  
  
tmp_target_dir <- file.path(tmp_dir, "kmers")  
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	<i>Converts a genome to kmers stored in libsvm format on disk</i>
------------------	---

Description

[Deprecated] This function converts a single genome to a libsvm file containing kmer counts. The libsvm 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.

Usage

```

genome_to_libsvm(
  x,
  target_path,
  label = "0",
  k = 3L,
  canonical = TRUE,
  squeeze = FALSE,
  overwrite = FALSE
)

genome_to_libsvm(
  x,
  target_path,
  label = "0",
  k = 3L,
  canonical = TRUE,
  squeeze = FALSE,
  overwrite = FALSE
)

```

Arguments

x	genome in string format
target_path	path to store libsvm file (.txt)
label	libsvm 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

Examples

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

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

Arguments

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

Value

vector containing MICs, or dataframe of IDs and MICs

Examples

```
df <- 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,
  prefer_high_mic = TRUE,
  simplify = TRUE)
```

kmers

Generates genome kmers

Description

[Deprecated]

Usage

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

```
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".

Examples

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

load_patric_db	<i>Load PATRIC database</i>
----------------	-----------------------------

Description

Load PATRIC database

Usage

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

Arguments

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

Value

PATRIC database (S3 class 'patric_db')

Examples

```
patric_db <- load_patric_db() # will get from PATRIC ftp
```

```
# make data.frame with single row
p <- data.frame(genome_id = 1,
                genome_name = "E. coli",
                antibiotic = "amoxicillin",
                measurement = 2.0,
                measurement_unit = "mg/L",
                laboratory_typing_method = "Agar dilution",
                resistant_phenotype = "R")
load_patric_db(p)
```

mic_censor	<i>Censor MIC values</i>
------------	--------------------------

Description

MIC datasets often arise from different laboratories or experimental conditions. In practice, this means that there can be different levels of censoring ($\leq$ 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

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

Value

censored MIC values (S3 `mic` class)

Examples

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

<code>mic_range</code>	<i>Generate dilution series</i>
------------------------	---------------------------------

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	<i>R breakpoint for MIC</i>
------------------	-----------------------------

Description

R breakpoint for MIC

Usage

```
mic_r_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 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	<i>S breakpoint for MIC</i>
------------------	-----------------------------

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

Examples

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

mic_uncensor	<i>Uncensor MICs</i>
--------------	----------------------

Description

Uncensor MICs

Usage

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


Arguments

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

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 ($\leq$) 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 package. 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*.

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	<i>Move or copy files using logical vector</i>
------------	--

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

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

Value

Logical vector, indicating success or failure for each file

Examples

```
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"),
    100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
}

# move files with even numbers to a new directory
new_dir <- file.path(tempdir(), "even_files")
unlink(new_dir, recursive = TRUE)
move_files(tmp_dir,
  new_dir,
  move_which = as.integer(
    tools::file_path_sans_ext(
      list.files(tmp_dir, pattern = "*.fna"))) %% 2 == 0,
  ext = ".fna")
list.files(new_dir)
```

plot.mic_validation *Plot MIC validation results*

Description

Plot MIC validation results

Usage

```
## S3 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

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)
```

```
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

Examples

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

```
print.mic_validation_summary
                          Print MIC validation summary
```

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))
```

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
)
```

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

```
pull_PATRIC_genomes(tempdir(),
                     taxonomic_name = "Escherichia coli",
                     filter = "MIC",
                     n_genomes = 10)
```

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"
)
```

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	<i>Check that QC measurement is at the required target</i> [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 alongside `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	<i>Reverse complement of DNA string</i>
--------------------	---

Description**[Deprecated]****Usage**

reverse_complement(dna)

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 `xgboost::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 directory)
names_backup	name of file to save backup of filename metadata (by default, will be names.csv 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

Examples

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

[Deprecated]

Usage

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

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

Arguments

x	integer vector of kmer indices
k	kmer length
starting_index	starting index (libsvm is usually indexed starting at 1)

Value

vector of squeezed kmer strings

Examples

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

squeezed_mers	<i>Generates all permutations of squeezed kmers</i>
---------------	---

Description

[Deprecated]

Usage

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

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

Arguments

k kmer length

Value

vector of squeezed kmers

Examples

```
squeezed_mers(3)
```

standardise_mic	<i>Standardise MIC to control strain</i> [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.

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
qc_measurement	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
ignore_na	Ignore NA (returns AMR::NA_mic_)
guideline	Guideline to use (EUCAST or CLSI)
year	Guideline year (version)
force	Force into MIC-compatible format after standardisation

Value

AMR::mic vector

Examples

```
# Ref strain QC MIC for GEN is 0.5
standardise_mic(
  test_measurement = c(AMR::as.mic(">8.0"), # QC = 1, censored MIC remains censored
                      AMR::as.mic(4.0), # QC = 0.5 which is on target, so stays same
                      AMR::as.mic(2), # QC = 1, so scaled down to 1
                      AMR::as.mic(2)), # QC = 0.25, so scaled up to 8
  qc_measurement = c(AMR::as.mic(1),
```

```

      AMR::as.mic(0.5),
      AMR::as.mic(1),
      AMR::as.mic(0.25)),
  strain = 25922,
  ab = AMR::as.ab("GEN"))

```

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 object
subset	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"))

```

summary.mic_validation	<i>Summary of MIC validation results</i>
------------------------	--

Description

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

Usage

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

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))
```

table	<i>Table</i>
-------	--------------

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",
  ...
)

```

Arguments

<code>x</code>	mic_validation S3 object
<code>...</code>	further arguments
<code>format</code>	simple or flextable
<code>fill_dilutions</code>	Fill dilutions that are not present in the data in order to match the y- and x- axes
<code>bold</code>	Bold cells where essential agreement is TRUE
<code>ea_color</code>	Background color for essential agreement cells
<code>gold_standard_name</code>	Name of the gold standard to display in output
<code>test_name</code>	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)

```

tidy_patric_meta_data *Tidy PATRIC data*

Description

Tidy PATRIC data

Usage

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

Arguments

<code>x</code>	PATRIC database loaded using <code>MIC::load_patric_db</code>
<code>prefer_more_resistant</code>	High MICs, narrow zones, or resistant phenotypes will be preferred where multiple reported for the same isolate
<code>as_ab</code>	convert antibiotics to <code>AMR::ab</code> class (column names are antibiotic codes)
<code>filter_abx</code>	filter antibiotics of interest, provided as a vector of antibiotics character names/codes, or ideally, as <code>AMR::ab</code> classes, created using <code>AMR::as.ab</code>

Value

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

Examples

```
db <- data.frame(genome_id = 1,
  genome_name = "E. coli",
  antibiotic = "amoxicillin",
  measurement = 2.0,
  measurement_unit = "mg/L",
  laboratory_typing_method = "Agar dilution",
  resistant_phenotype = "R")
db <- load_patric_db(db)
tidy_patric_meta_data(db)
```

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()
# 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,
  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

[Deprecated]

Usage

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

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

Arguments

x	integer vector of kmer indices
k	kmer length
starting_index	starting index (libsvm is usually indexed starting at 1)

Value

vector of unsqueezed kmer strings

Examples

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

`unsqueezed_mers`*Generates all permutations of unsqueezed kmers*

Description

[Deprecated]

Usage

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

```
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 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 `xgboost::xgb.cv`, but can be desirable if there is downstream processing that depends on an `xgb.cv.synchronous` 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.

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

params	parameters for xgboost
data	DMatrix or matrix
nrounds	number of training rounds
nfold	number of folds, or if < 1 then the proportion will be used as the training split in a train-test split
label	data labels (alternatively provide with DMatrix)
missing	handling of missing data (see xgb.cv)
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	print every n iterations
early_stopping_rounds	early stopping rounds (applied to each fold)
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

Examples

```

train <- list(data = matrix(rnorm(20), ncol = 2),
              label = rbinom(10, 1, 0.5))
dtrain <- xgboost::xgb.DMatrix(train$data, label = train$label, nthread = 1)
cv <- xgb.cv.lowmem(data = dtrain,

```

```
params = list(objective = "binary:logistic"),  
nrounds = 2,  
nfold = 3,  
prediction = TRUE,  
nthread = 1)
```

cv

Index

- * **datasets**
 - ecoffs, [10](#)
 - example_mics, [12](#)
- as.sir_vectorised, [3](#)
- bias, [4](#)
- clean_raw_mic, [4](#)
- combined_file_system, [5](#)
- compare_mic, [6](#)
- compare_sir, [8](#)
- download_patric_db, [8](#)
- droplevels.mic_validation, [9](#)
- ecoffs, [10](#)
- essential_agreement, [7](#), [11](#)
- example_mics, [12](#)
- fill_dilution_levels, [13](#)
- force_mic, [12](#), [14](#)
- genome_to_libsvm, [17](#)
- genome_to_libsvm(), [16](#)
- genomes_to_kmer_libsvm, [15](#)
- genomes_to_kmer_libsvm(), [18](#)
- get_mic, [18](#)
- kmers, [19](#)
- load_patric_db, [21](#)
- mic_censor, [21](#)
- mic_r_breakpoint, [23](#)
- mic_range, [22](#)
- mic_s_breakpoint, [24](#)
- mic_uncensor, [12](#), [24](#)
- move_files, [26](#)
- plot.mic_validation, [27](#)
- print.mic_validation, [28](#)
- print.mic_validation_summary, [28](#)
- pull_PATRIC_genomes, [29](#)
- qc_in_range, [30](#)
- qc_on_target, [31](#)
- replace_multiple_slashes, [32](#)
- reverse_complement, [33](#)
- split_and_combine_files, [33](#)
- split_and_combine_files(), [16](#)
- squeezed_index_to_str, [35](#)
- squeezed_mers, [36](#)
- standardise_mic, [36](#)
- subset.mic_validation, [38](#)
- summary.mic_validation, [39](#)
- table, [39](#)
- tidy_patric_meta_data, [40](#)
- train_test_filesystem, [41](#)
- unsqueezed_index_to_str, [43](#)
- unsqueezed_mers, [43](#)
- with_progress, [15](#)
- xgb.cv.lowmem, [44](#)