

Package ‘CellBench’

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Type Package

Title Construct Benchmarks for Single Cell Analysis Methods

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Description This package contains infrastructure for benchmarking analysis methods and access to single cell mixture benchmarking data. It provides a framework for organising analysis methods and testing combinations of methods in a pipeline without explicitly laying out each combination. It also provides utilities for sampling and filtering SingleCellExperiment objects, constructing lists of functions with varying parameters, and multithreaded evaluation of analysis methods.

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URL <https://github.com/shians/cellbench>

BugReports <https://github.com/Shians/CellBench/issues>

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CellBench-package	<i>A framework for benchmarking combinations of methods in multi-stage pipelines</i>
-------------------	--

Description

This package contains a framework for benchmarking combinations of methods in a multi-stage pipeline. It is mainly based around the `apply_methods` function, which takes lists of functions to be applied in stages of a pipeline.

Author(s)

Shian Su <<https://www.github.com/shians>>

See Also

The core function in this package is `apply_methods`, see `vignette("Introduction", package = "CellBench")` for basic usage. Run `cellbench_case_study()` to see a case study using CellBench. The data loading functions from `load_all_data` may also be of interest.

<code>all_unique</code>	<i>Check if all values in a vector are unique</i>
-------------------------	---

Description

Check if all values in a vector are unique

Usage

```
all_unique(x)
```

Arguments

`x` the vector to check

Value

TRUE if all values in the vector are unique

Examples

```
all_unique(c(1, 2, 3)) # TRUE
all_unique(c(1, 2, 2)) # FALSE
```

any_task_errors	<i>Check if any tasks produced errors</i>
-----------------	---

Description

Check the results column of a benchmark tibble for any task_error objects.

Usage

```
any_task_errors(x, verbose)

## S3 method for class 'benchmark_tbl'
any_task_errors(x, verbose = FALSE)
```

Arguments

x	the tibble to check
verbose	TRUE if the rows with errors should be reported

Value

TRUE if any entry in the result column is a task_error object

Methods (by class)

- any_task_errors(benchmark_tbl):

apply_methods	<i>Apply methods</i>
---------------	----------------------

Description

apply_methods() and its aliases apply_metrics and begin_benchmark take either lists of datasets or benchmark_tbl objects and applies a list of functions. The output is a benchmark_tbl where each method has been applied to each dataset or preceding result.

Usage

```
apply_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

## S3 method for class 'list'
apply_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

## S3 method for class 'benchmark_tbl'
apply_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

## S3 method for class 'tbl_df'
apply_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

apply_metrics(x, fn_list, name = NULL, suppress.messages = TRUE)

begin_benchmark(x, fn_list, name = NULL, suppress.messages = TRUE)
```

Arguments

x the list of data or benchmark tibble to apply methods to
fn_list the list of methods to be applied
name (optional) the name of the column for methods applied
suppress.messages TRUE if messages from running methods should be suppressed

Value

benchmark_tbl object containing results from methods applied, the first column is the name of the dataset as factors, middle columns contain method names as factors and the final column is a list of results of applying the methods.

See Also

[time_methods](#)

Examples

```

# list of data
datasets <- list(
  set1 = rnorm(500, mean = 2, sd = 1),
  set2 = rnorm(500, mean = 1, sd = 2)
)

# list of functions
add_noise <- list(
  none = identity,
  add_bias = function(x) { x + 1 }
)

res <- apply_methods(datasets, add_noise)

```

arrow_sep

Unicode arrow separators

Description

Utility function for generating unicode arrow separators.

Usage

```
arrow_sep(towards = c("right", "left"), unicode = FALSE)
```

Arguments

towards the direction the unicode arrow points towards
unicode whether unicode arrows should be used. Does not work inside plots within knitted PDF documents.

Value

a string containing an unicode arrow surrounded by two spaces

Examples

```
arrow_sep("left") # left arrow
arrow_sep("right") # right arrow
```

as_pipeline_list	<i>convert benchmark_tbl to list</i>
------------------	--------------------------------------

Description

convert a benchmark_tbl to a list where the name of the elements represent the pipeline steps separated by "..". This can be useful for using the apply family of functions.

Usage

```
as_pipeline_list(x)
```

Arguments

x the benchmark_tbl object to convert

Value

list containing the results with names set to data and pipeline steps separated by ..

See Also

[collapse_pipeline](#)

Examples

```
# list of data
datasets <- list(
  set1 = rnorm(500, mean = 2, sd = 1),
  set2 = rnorm(500, mean = 1, sd = 2)
)

# list of functions
add_noise <- list(
  none = identity,
  add_bias = function(x) { x + 1 }
)

res <- apply_methods(datasets, add_noise)
as_pipeline_list(res)
```

cache_method	<i>Create a cached function for CellBench</i>
--------------	---

Description

Take a function and return a cached version. The arguments and results of a cached method is saved to disk and if the cached function is called again with the same arguments then the results will be retrieved from the cache rather than be recomputed.

Usage

```
cache_method(f, cache = getOption("CellBench.cache"))
```

Arguments

f	the function to be cached
cache	the cache information (from memoise package)

Details

(CAUTION) Because cached functions called with the same argument will always return the same output, pseudo-random methods will not return varying results over repeated runs as one might expect.

This function is a thin wrapper around [memoise](#)

Value

function whose results are cached and is called identically to f

See Also

[set_cellbench_cache_path](#)

Examples

```
# sets cache path to a temporary directory
set_cellbench_cache_path(file.path(tempdir(), ".CellBenchCache"))
f <- function(x) { x + 1 }
cached_f <- cache_method(f)
```

cellbench_case_study *Open vignette containing a case study using CellBench*

Description

Open vignette containing a case study using CellBench

Usage

```
cellbench_case_study()
```

Value

opens a vignette containing a case study

Examples

```
## Not run:  
cellbench_case_study()  
  
## End(Not run)
```

cellbench_file *Get path to CellBench packaged data*

Description

Search CellBench package for packaged data, leaving argument empty will list the available data.

Usage

```
cellbench_file(filename = NULL)
```

Arguments

filename the name of the file to look for

Value

string containing the path to the packaged data

Examples

```
cellbench_file() # shows available files  
cellbench_file("10x_sce_sample.rds") # returns path to 10x sample data
```

check_class	<i>Check class of object</i>
-------------	------------------------------

Description

Check an object against a vector of class names. Testing if they match any or all of the classes. For `is_all_of`, the object needs to be at least every class specified, but it can have addition classes and still pass the check.

Usage

```
is_one_of(x, classes)
```

```
is_any_of(x, classes)
```

```
is_all_of(x, classes)
```

Arguments

x	the object to check
classes	the vector of strings of class names

Value

boolean value for the result of the check

Examples

```
is_one_of(1, c("numeric", "logical")) # TRUE
is_one_of(1, c("character", "logical")) # FALSE

is_all_of(1, c("numeric", "logical")) # FALSE
is_all_of(tibble::tibble(), c("tbl", "data.frame")) # TRUE
```

clear_cached_datasets	<i>Clear cached datasets</i>
-----------------------	------------------------------

Description

Delete the datasets cached by the `load_*_data` set of functions

Usage

```
clear_cached_datasets()
```

Value

None

Examples

```
## Not run:
clear_cached_datasets()

## End(Not run)
```

clear_cellbench_cache *Clear CellBench Cache*

Description

Clears the method cache for CellBench

Usage

```
clear_cellbench_cache()
```

Value

None

Examples

```
## Not run:
clear_cellbench_cache()

## End(Not run)
```

collapse_pipeline *Collapse benchmark_tbl into a two column summary*

Description

Collapse benchmark_tbl into two columns: "pipeline" and "result". The "pipeline" column will be the concatenated values from the data and methods columns while the "result" column remains unchanged from the benchmark_tbl. This is useful for having a string summary of the pipeline for annotating.

Usage

```
collapse_pipeline(
  x,
  sep = arrow_sep("right"),
  drop.steps = TRUE,
  data.name = TRUE
)

pipeline_collapse(
  x,
```

```

    sep = arrow_sep("right"),
    drop.steps = TRUE,
    data.name = TRUE
  )

```

Arguments

x	the benchmark_tbl to collapse
sep	the separator to use for concatenating the pipeline steps
drop.steps	if the data name and methods steps should be dropped from the output. TRUE by default.
data.name	if the dataset name should be included in the pipeline string. Useful if only a single dataset is used.

Value

benchmark_tbl with pipeline and result columns (and all other columns if drop.steps is FALSE)

See Also

[as_pipeline_list](#)

Examples

```

# list of data
datasets <- list(
  set1 = rnorm(500, mean = 2, sd = 1),
  set2 = rnorm(500, mean = 1, sd = 2)
)

# list of functions
add_noise <- list(
  none = identity,
  add_bias = function(x) { x + 1 }
)

res <- apply_methods(datasets, add_noise)
collapse_pipeline(res)

```

data_list

Constructor for a data list

Description

Constructor for a list of data, a thin wrapper around list() which checks that all the inputs are of the same type and have names

Usage

```
data_list(...)
```

Arguments

... objects, must all be named

Value

a list of named data

Examples

```
data(iris)
flist <- data_list(
  data1 = iris[1:20, ],
  data2 = iris[21:40, ]
)
```

filter_zero_genes *Filter out zero count genes*

Description

Remove all genes (rows) where the total count is 0

Usage

```
filter_zero_genes(x)
```

Arguments

x the SingleCellExperiment or matrix to filter

Value

object of same type as input with all zero count genes removed

Examples

```
x <- matrix(rep(0:5, times = 5), nrow = 6, ncol = 5)
filter_zero_genes(x)
```

fn_arg_seq	<i>Create a list of functions with arguments varying over a sequence</i>
------------	--

Description

Generate a list of functions where specific arguments have been pre-applied from a sequences of arguments, i.e. a function $f(x, n)$ may have the 'n' argument pre-applied with specific values to obtain functions $f_1(x, n = 1)$ and $f_2(x, n = 2)$ stored in a list.

Usage

```
fn_arg_seq(func, ..., .strict = FALSE)
```

Arguments

func	function to generate list from
...	vectors of values to use as arguments
.strict	TRUE if argument names are checked, giving an error if specified argument does not appear in function signature. Note that functions with multiple methods generally have only $f(x, \dots)$ as their signature, so the check would fail even if the arguments are passed on.

Details

If multiple argument vectors are provided then the combinations of arguments in the sequences will be generated.

Value

list of functions with the specified arguments pre-applied. Names of the list indicate the values that have been pre-applied.

Examples

```
f <- function(x) {
  cat("x:", x)
}

f_list <- fn_arg_seq(f, x = c(1, 2))
f_list
f_list[[1]]() # x: 1
f_list[[2]]() # x: 2

g <- function(x, y) {
  cat("x:", x, "y:", y)
}

g_list <- fn_arg_seq(g, x = c(1, 2), y = c(3, 4))
g_list
g_list[[1]]() # x: 1 y: 3
g_list[[2]]() # x: 1 y: 4
g_list[[3]]() # x: 2 y: 3
g_list[[4]]() # x: 2 y: 4
```

fn_list	<i>Constructor for a function list</i>
---------	--

Description

Constructor for a list of functions, a thin wrapper around list() which checks that all the inputs are functions and have names

Usage

```
fn_list(...)
```

Arguments

... objects, must all be named

Value

a list of named functions

Examples

```
flist <- fn_list(  
  mean = mean,  
  median = median  
)
```

is.task_error	<i>Check for task errors</i>
---------------	------------------------------

Description

This is a helper function for checking the result column of a benchmark_tbl for task_error objects. This is useful for filtering out rows where the result is a task error.

Usage

```
is.task_error(x)
```

Arguments

x the object to be tested

Value

vector of logicals denoting if elements of the list are task_error objects

keep_high_count_cells *Filter down to the highest count cells*

Description

Filter a SingleCellExperiment or matrix down to the cells (columns) with the highest counts

Usage

```
keep_high_count_cells(x, n)
```

Arguments

x the SingleCellExperiment or matrix
n the number of highest count cells to keep

Value

object of same type as input containing the highest count cells

Examples

```
data(sample_sce_data)  
keep_high_count_cells(sample_sce_data, 10)
```

keep_high_count_genes *Filter down to the highest count genes*

Description

Filter a SingleCellExperiment or matrix down to the genes (rows) with the highest counts

Usage

```
keep_high_count_genes(x, n)
```

Arguments

x the SingleCellExperiment or matrix
n the number of highest count genes to keep

Value

object of same type as input containing the highest count genes

Examples

```
data(sample_sce_data)  
keep_high_count_genes(sample_sce_data, 300)
```

keep_high_var_genes *Filter down to the most variable genes*

Description

Filter a SingleCellExperiment or matrix down to the most variable genes (rows), variability is determined by var() scaled by the total counts for the gene.

Usage

```
keep_high_var_genes(x, n)
```

Arguments

x the SingleCellExperiment or matrix
n the number of most variable genes to keep

Value

object of same type as input containing the most variable genes

Examples

```
data(sample_sce_data)  
keep_high_var_genes(sample_sce_data, 50)
```

load_sc_data *Load CellBench Data*

Description

Load in all CellBench data described at <https://github.com/LuyiTian/CellBench_data/blob/master/README.md>.

Usage

```
load_sc_data()  
  
load_cell_mix_data()  
  
load_mrna_mix_data()  
  
load_all_data()
```

Value

list of SingleCellExperiment

Functions

- `load_sc_data()`: Load single cell data
- `load_cell_mix_data()`: Load cell mixture data
- `load_mrna_mix_data()`: Load mrna mixture data

Examples

```
## Not run:  
cellbench_file <- load_all_data()  
  
## End(Not run)
```

mhead

Get head of 2 dimensional object as a square block

Description

head prints all columns which may flood the console, mhead takes a square block which can look nicer and still provide a good inspection of the contents

Usage

```
mhead(x, n = 6)
```

Arguments

x the object with 2 dimensions
n the size of the n-by-n block to extract

Value

an n-by-n sized subset of x

Examples

```
x <- matrix(runif(100), nrow = 10, ncol = 10)  
  
mhead(x)  
mhead(x, n = 3)
```

`print.fn_arg_seq` *Print method for fn_arg_seq output*

Description

Print method for `fn_arg_seq` output

Usage

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

Arguments

`x` `fn_arg_seq` object
`...` addition arguments for `print`

Value

None

Examples

```
fn_seq <- fn_arg_seq(kmeans, centers = 1:3)  
fn_seq
```

`print.task_error` *Print method for task_error object*

Description

`task_error` are objects that result from failed methods

Usage

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

Arguments

`x` a `task_error` object
`...` not used

Value

None

sample_cells	<i>Sample cells from a SingleCellExperiment</i>
--------------	---

Description

Sample n cells from a SingleCellExperiment object with no replacement.

Usage

```
sample_cells(x, n)
```

Arguments

x	the SingleCellExperiment object
n	the number of cells to sample

Value

SingleCellExperiment object

Examples

```
sample_sce_data <- readRDS(cellbench_file("celseq_sce_sample.rds"))
dim(sample_sce_data)
x <- sample_cells(sample_sce_data, 10)
dim(x)
```

sample_genes	<i>Sample genes from a SingleCellExperiment</i>
--------------	---

Description

Sample n genes from a SingleCellExperiment object with no replacement

Usage

```
sample_genes(x, n)
```

Arguments

x	the SingleCellExperiment object
n	the number of genes to sample

Value

SingleCellExperiment object

Examples

```
sample_sce_data <- readRDS(cellbench_file("10x_sce_sample.rds"))
dim(sample_sce_data)
x <- sample_genes(sample_sce_data, 50)
dim(x)
```

sample_sce_data	<i>This is data for testing functions in CellBench.</i>
-----------------	---

Description

A dataset containing 200 genes and 50 cells randomly sampled from the CelSeq mRNA mixture dataset, each sample is a mixture of mRNA material from 3 different human adenocarcinoma cell lines. Useful for quick prototyping of method wrappers.

Usage

```
data(sample_sce_data)
```

Format

A SingleCellExperiment object with sample annotations in `colData(sample_sce_data)`. The annotation contains various QC metrics as well as the cell line mixture proportions

H2228_prop proportion of mRNA from H2228 cell line

H1975_prop proportion of mRNA from H1975 cell line

HCC827_prop proportion of mRNA from HCC827 cell line

See Also

[load_mrna_mix_data](#)

set_cellbench_bpparam	<i>Set BiocParallel parameter used CellBench</i>
-----------------------	--

Description

This is a more advanced interface for changing CellBench's parallelism settings. Internally CellBench uses BiocParallel for parallelism, consult the documentation of BiocParallel to see what settings are available.

Usage

```
set_cellbench_bpparam(param)
```

Arguments

param the BiocParallel parameter object

Value

None

See Also

[set_cellbench_threads](#) for more basic interface

Examples

```
set_cellbench_threads(1) # CellBench runs on a single thread
```

```
set_cellbench_cache_path  
    Set CellBench cache path
```

Description

Set CellBench cache path

Usage

```
set_cellbench_cache_path(path = "./.CellBenchCache")
```

Arguments

path the path to where method caches should be stored

Value

None

See Also

[cache_method](#) for constructing cached methods.

Examples

```
## Not run:  
# hidden folder in local path  
set_cellbench_cache_path("./.CellBenchCache")  
  
## End(Not run)  
# store in temp directory valid for this session  
set_cellbench_cache_path(file.path(tempdir(), ".CellBenchCache"))
```

```
set_cellbench_threads    Set number of threads used by CellBench
```

Description

Sets global parameter for CellBench to use multiple threads for applying methods. If any methods applied are multi-threaded then it's recommended to set CellBench threads to 1. It only recommended to use CellBench with multiple threads if methods applied can be set to run on single threads.

Usage

```
set_cellbench_threads(nthreads = 1)
```

Arguments

nthreads the number of threads used by CellBench

Value

None

See Also

[set_cellbench_bpparam](#) for more advanced interface

Examples

```
set_cellbench_threads(1) # CellBench runs on a single thread
```

split_step	<i>Split combined pipeline step</i>
------------	-------------------------------------

Description

Some methods perform multiple steps of a pipeline. This function assists with splitting the combined pipeline step into multiple steps with duplicated method names.

Usage

```
split_step(x, step, into)
```

Arguments

x a results data.frame from 'apply_methods()'.
step the name of the column to split.
into the name of the columns to split into.

Value

a results data.frame where the 'step' column has been split into the 'into' columns with duplicated values.

Examples

```
datasets <- list(
  set1 = rnorm(500, mean = 2, sd = 1),
  set2 = rnorm(500, mean = 1, sd = 2)
)

# list of functions
add_noise <- list(
  none = identity,
  add_bias = function(x) { x + 1 }
)

res <- apply_methods(datasets, add_noise)

res %>%
  split_step("add_noise", c("split1", "split2"))
```

strip_timing

Strip timing information

Description

Takes the result of a `time_methods()` call and remove timing information from the ‘`timed_result`’ column, replacing it with a ‘`result`’ column and converting it to a `benchmark_tbl`.

Usage

```
strip_timing(x)

## S3 method for class 'benchmark_timing_tbl'
strip_timing(x)
```

Arguments

`x` the `benchmark_timing_tbl` object

Value

`benchmark_tbl`

See Also

[unpack_timing](#)

Examples

```
## Not run:
datasets <- list(
  data1 = 1:1e8,
)

transforms <- list(
  log = log,
```

```
    sqrt = sqrt
  )

  datasets %>%
    time_methods(transforms) %>%
    strip_timing()

## End(Not run)
```

summary.benchmark_tbl *Summary of benchmark_tbl*

Description

Summary of benchmark_tbl

Usage

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

Arguments

object	the benchmark_tbl to be summarised
...	additional arguments affecting the summary produced.

Value

None

Examples

```
# list of data
datasets <- list(
  set1 = rnorm(500, mean = 2, sd = 1),
  set2 = rnorm(500, mean = 1, sd = 2)
)

# list of functions
add_noise <- list(
  none = identity,
  add_bias = function(x) { x + 1 }
)

res <- apply_methods(datasets, add_noise)
summary(res)
```

time_methods	<i>Time methods</i>
--------------	---------------------

Description

`time_methods()` take either lists of datasets or `benchmark_timing_tbl` objects and applies a list of functions. The output is a `benchmark_timing_tbl` where each method has been applied to each dataset or preceding result. Unlike `apply_methods()`, `time_methods()` is always single threaded as to produce fair and more consistent timings.

Usage

```
time_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

## S3 method for class 'list'
time_methods(x, fn_list, name = NULL, suppress.messages = TRUE)

## S3 method for class 'benchmark_timing_tbl'
time_methods(x, fn_list, name = NULL, suppress.messages = TRUE)
```

Arguments

<code>x</code>	the list of data or benchmark timing tibble to apply methods to
<code>fn_list</code>	the list of methods to be applied
<code>name</code>	(optional) the name of the column for methods applied
<code>suppress.messages</code>	TRUE if messages from running methods should be suppressed

Value

`benchmark_timing_tbl` object containing results from methods applied, the first column is the name of the dataset as factors, middle columns contain method names as factors and the final column is a list of lists containing the results of applying the methods and timings from calling `system.time()`.

See Also

[apply_methods](#)

Examples

```
datasets <- list(
  set1 = 1:1e7
)

transform <- list(
  sqrt = sqrt,
  log = log
)

time_methods(datasets, transform) %>%
  unpack_timing() # extract timings out of list
```

unpack_timing	<i>Unpack timing information</i>
---------------	----------------------------------

Description

Takes the result of a `time_methods()` call and remove the 'timed_result' column, replacing it with three columns of durations representing the 'system', 'user' and 'elapsed' times from a `system.time()` call.

Usage

```
unpack_timing(x)

## S3 method for class 'benchmark_timing_tbl'
unpack_timing(x)
```

Arguments

x the benchmark_timing_tbl object

Value

a tibble containing pipeline steps and timing information

See Also

[strip_timing](#)

Examples

```
## Not run:
datasets <- list(
  data1 = c(1, 2, 3)
)

transforms <- list(
  log = function(x) { Sys.sleep(0.1); log(x) },
  sqrt = function(x) { Sys.sleep(0.1); sqrt(x) }
)

datasets %>%
  time_methods(transforms) %>%
  unpack_timing()

## End(Not run)
```

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