Package ‘CellBench’

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Type Package

Title Construct Benchmarks for Single Cell Analysis Methods

Version 1.20.0

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.

biocViews Software, Infrastructure, SingleCell

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

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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.

---

**all_unique**

*Check if all values in a vector are unique*

## 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

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

---

any_task_errors  

*Check if any tasks produced errors*

---

**Description**

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

**Usage**

```r
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  

*Apply methods*

---

**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 preceeding result.

**Usage**

```r
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'

```r
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

```r
# 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**  
*convert benchmark_tbl to list*

**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

```r
# 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

Create a cached function for CellBench

#### 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

```r
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)

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)

Description

Get path to CellBench packaged data

Usage

cellbench_file(filename = NULL)
check_class

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

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 additional 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  Clear cached datasets

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

```r
# 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

```r
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
Create a list of functions with arguments varying over a sequence

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 f1(x, n = 1) and f2(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, ...) 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

```r
f <- function(x) {
  cat("x:", x)
}
n_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  
Constructor for a function list

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

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

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

```r
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

```r
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
**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**
```r
keep_high_var_genes(x, n)
```

**Arguments**
- `x` the SingleCellExperiment or matrix
- `n` the number of most variable genes to keep

**Examples**
```r
data(sample_sce_data)
keep_high_var_genes(sample_sce_data, 300)
```
**load_sc_data**

**Value**

object of same type as input containing the most variable genes

**Examples**

```r
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**

```r
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**

```r
## 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
```

---

Sample cells from a SingleCellExperiment

**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)

dimensions

Sample genes from a SingleCellExperiment

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

This is data for testing functions in CellBench.

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  Set BiocParallel parameter used CellBench

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

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

---

`set_cellbench_cache_path`

*Set CellBench cache path*

Description

Set CellBench cache path

Usage

```r
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

```r
## 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**  
*Split combined pipeline step*

**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.
to 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
summary.benchmark_tbl

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)
Examples

```r
# 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**

**Time methods**

**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**

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

**Arguments**

- `x` the list of data or benchmark timing tbl 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_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().
unpack_timing

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

Unpack timing information

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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