Package 'struct'

March 26, 2024

Type Package

Title Statistics in R Using Class-based Templates

Version 1.14.1

Description Defines and includes a set of class-based templates for developing
and implementing data processing and analysis workflows, with a strong
emphasis on statistics and machine learning. The templates can be used and
where needed extended to 'wrap' tools and methods from other packages into a
common standardised structure to allow for effective and fast integration.
Model objects can be combined into sequences, and sequences nested in
iterators using overloaded operators to simplify and improve readability of
the code. Ontology lookup has been integrated and implemented
to provide standardised definitions for methods, inputs and outputs wrapped
using the class-based templates.

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Encoding UTF-8

Collate 'generics.R' 'ontology_term_class.R' 'struct_class.R'
'parameter_class.R' 'chart_class.R' 'stato_class.R'
'DatasetExperiment_class.R' 'entity_class.R'
'entity_stato_class.R' 'enum_class.R' 'enum_stato_class.R'
'output_class.R' 'model_class.R' 'example_objects.R'
'model_list_class.R' 'metric_class.R' 'iterator_class.R'
'optimiser_class.R' 'preprocess_class.R' 'resampler_class.R'
'struct.R' 'struct_templates.R'

RoxygenNote 7.3.1

Depends R (>= 4.0)

Suggests testthat, rstudioapi, rmarkdown, covr, BiocStyle, openxlsx,
ggplot2, magick

VignetteBuilder knitr

Imports methods, ontologyIndex, datasets, graphics, stats, utils,
knitr, SummarizedExperiment, S4Vectors, rols (>= 2.30.1)

biocViews WorkflowStep

git_url https://git.bioconductor.org/packages/struct

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R **topics documented:**

.DollarNames.struct_class

autocompletion

Description

This function returns slotnames for autocompletion when using $ syntax

Usage

```
## S3 method for class 'struct_class'
.DollarNames(x, pattern = "")

## S4 method for signature 'struct_class'
.DollarNames(x, pattern = "")

## S3 method for class 'chart'
.DollarNames(x, pattern = "")

## S4 method for signature 'chart'
.DollarNames(x, pattern = "")

## S3 method for class 'DatasetExperiment'
.DollarNames(x, pattern = "")

## S4 method for signature 'DatasetExperiment'
.DollarNames(x, pattern = "")

## S3 method for class 'model'
.DollarNames(x, pattern = "")

## S4 method for signature 'model'
.DollarNames(x, pattern = "")

## S3 method for class 'metric'
.DollarNames(x, pattern = "")

## S4 method for signature 'metric'
.DollarNames(x, pattern = "")

## S3 method for class 'iterator'
.DollarNames(x, pattern = "")

## S4 method for signature 'iterator'
.DollarNames(x, pattern = "")

## S3 method for class 'optimiser'
.DollarNames(x, pattern = "")

## S4 method for signature 'optimiser'
.DollarNames(x, pattern = "")

## S3 method for class 'preprocess'
.DollarNames(x, pattern = "")

## S4 method for signature 'preprocess'
.DollarNames(x, pattern = "")
```

```
## S3 method for class 'resampler'
.DollarNames(x, pattern = "")

## S4 method for signature 'resampler'
.DollarNames(x, pattern = "")
```

Arguments

x	a struct_class object
pattern	the text used to compare against the slot names

Value

A vector of slot names

---

as.code *Convert to code*

Description

Prints a block of code that can be used to replicate the input object.

Usage

```
as.code(M, start = "M = ", mode = "compact", quiet = FALSE)

## S4 method for signature 'struct_class'
as.code(M, start = "M = ", mode = "compact", quiet = FALSE)

## S4 method for signature 'model_seq'
as.code(M, start = "M = ", mode = "compact", quiet = FALSE)

## S4 method for signature 'iterator'
as.code(M, start = "M = ", mode = "compact", quiet = FALSE)
```

Arguments

M	a struct model, model_seq or iterator object
start	text prepended to the code. Default is "M = "
mode	"compact" will use the least amount of lines, "expanded" will put each object and input on a new line. "neat" will produce an output somewhere between "compact" and "expanded".
quiet	TRUE or FALSE to print code to console

Value

A string of code to reproduce the input object.

a string of code to reproduce the model

a string of code to reproduce the model sequence

a string of code to reproduce the iterator

Examples

```
M = example_model(value_1 = 10)
as.code(M)
M = example_model()
as.code(M)
M = example_model()
as.code(M)
M = example_model()
as.code(M)
```

---

as.DatasetExperiment   *Convert a SummarizedExperiment to DatasetExperiment*

Description

Converts a SummarizedExperiment to DatasetExperiment. The assay data is transposed, and col-
Data and rowData switched to match. struct specific slots such as "name" and "description" are
extracted from the metaData.

Usage

```
as.DatasetExperiment(obj)
```

Arguments

obj   a SummarizedExperiment object

Value

a DatasetExperiment object

---

as.DatasetExperiment,SummarizedExperiment-method

Convert a SummarizedExperiment to DatasetExperiment

Description

The assay data is transposed, and colData and rowData switched to match. struct specific slots such as "name" and "description" are extracted from the metaData if available. NB Any additional metadata will be lost during this conversion.

Usage

```
## S4 method for signature 'SummarizedExperiment'
as.DatasetExperiment(obj)
```

Arguments

obj   a SummarizedExperiment object

Value

a DatasetExperiment object

---

as.SummarizedExperiment

Convert a DatasetExperiment to a SummarizedExperiment

Description

Converts a DatasetExperiment to SummarizedExperiment. The assay data is transposed, and colData and rowData switched to match. struct specific slots such as "name" and "description" are stored in the metaData.

Usage

```
as.SummarizedExperiment(obj)
```

Arguments

obj   a DatasetExperiment object

Value

a SummarizedExperiment object

`as.SummarizedExperiment,DatasetExperiment-method`

Convert a DatasetExperiment to SummarizedExperiment

Description

Converts a DatasetExperiment to SummarizedExperiment. The assay data is transposed, and colData and rowData switched to match. struct specific slots such as "name" and "description" are stored in the metaData.

Usage

```
## S4 method for signature 'DatasetExperiment'
as.SummarizedExperiment(obj)
```

Arguments

obj   a DatasetExperiment object

Value

a SummarizedExperiment object

`as_data_frame`   *convert to data.frame*

Description

Most often used with univariate statistics to gather all the different outputs in a consistent format.

Usage

```
as_data_frame(M, ...)
```

Arguments

M   a struct object

...   other inputs passed through this function

Value

a data.frame containing outputs from an object

`c,ontology_list-method`

catenate ontology_lists

Description

ontology_lists can be catenated with other ontology lists or with ontology_items.

Usage

```
## S4 method for signature 'ontology_list'
c(x, ...)
```

Arguments

x   an ontology_list()

...   any number of ontology_list() or ontology_item() objects to catenate

Value

an ontology_list()

---

calculate   *Calculate metric*

Description

A class for metrics to assess performance of e.g. models, iterators. Not intended to be called directly, this class should be inherited to provide functionality for method-specific classes.

Usage

```
calculate(obj, ...)

value(obj)

value(obj) <- value

max_length(obj) <- value

metric(...)

## S4 method for signature 'metric'
calculate(obj, Y, Yhat)
```

```
## S4 method for signature 'metric'
value(obj)

## S4 replacement method for signature 'metric'
value(obj) <- value
```

Arguments

obj	a metric object
...	named slots and their values.
value	value
Y	the true class labels
Yhat	the predicted class labels

Value

value the calculated value of a metric

a metric object

Examples

```
MET = metric()
calculate(MET)
MET = metric()
M = metric()
calculate(M,Y,Yhat)
MET = metric()
value(MET)
MET = metric()
value(MET) = 10
```

---

chart   *Constructor for struct chart objects*

Description

A base class in the **struct** package. Should not be called directly.

Usage

```
chart(...)
```

Arguments

...	named slots and their values that get passed to struct_class

Details

The chart class provides a template for figures, charts and plots associated with other objects. For example, a DatasetExperiment object could have a histogram plotted for a specified column.

Charts can have parameters but not outputs (other than the figure itself), as chart objects are not intended to be used for calculations. The chart_plot method can be used to display a chart for an object, and chart_names can be used to list all chart objects associated with an object.

Classes that inherit the stato class have STATO integration enabled, allowing stato_id to be set and formal names and descriptions pulled from the STATO ontology database.

Value

a chart object

a struct_class object

Examples

```
C = example_chart()
```

---

chart_names   *chart names*

Description

Returns a list of valid charts for a struct object

Usage

```
chart_names(obj, ret = "char")

## S4 method for signature 'struct_class'
chart_names(obj, ret = "char")
```

Arguments

obj	An object derived from the struct_class object
ret	A string indicating whether a list of objects ('obj') or a list of chart names ('char') is returned. 'char' is default.

Details

The chart_names method searches chart objects that specify the input object type as an input.

Value

list of chart names, or a list of chart objects

Methods (by class)

- struct_class:

Examples

```
M = example_model()
chart_names(M) # 'example_chart'
chart_names(M,'char') # as above
chart_names(M,'obj') # returns a list of chart objects
```

---

chart_plot   *chart_plot*

Description

Plots a chart object

Usage

```
chart_plot(obj, dobj, ...)

## S4 method for signature 'chart,ANY'
chart_plot(obj, dobj)
```

Arguments

obj	A chart object
dobj	An object derived from struct_class
...	optional inputs

Details

The optional optional inputs depend on the input object/chart, but might include an additional dataset object or a second model object, for example.

Value

a plot object

Methods (by class)

- obj = chart,dobj = ANY:

Examples

```
C = example_chart()
chart_plot(C,iris_DatasetExperiment())
```

---

citations   *Citations for an object*

Description

All `struct` objects have a "citations" slot, which is a list of references in bibtex format. The `citations` method gathers citations from an object and all `struct` objects that it inherits to generate a complete list.

Usage

```
citations(obj)

## S4 method for signature 'struct_class'
citations(obj)
```

Arguments

obj   a struct object

Value

a character array of citations

Examples

```
D = iris_DatasetExperiment()
D$citations # the list specifically defined for this object
citations(D) # the list for this object and all inherited ones
```

DatasetExperiment   *DatasetExperiment class*

Description

An object for holding raw data and associated meta data

Usage

```
DatasetExperiment(
  data = data.frame(),
  sample_meta = data.frame(),
  variable_meta = data.frame(),
  ...
)
```

```
## S4 method for signature 'DatasetExperiment'
x$name

## S4 replacement method for signature 'DatasetExperiment'
x$name <- value
```

Arguments

data	A data frame with samples in rows and features in columns
sample_meta	A data frame with samples in rows and meta data in columns
variable_meta	A data frame with features in rows and meta data in columns
...	named slot values to pass through to struct_class
x	A DatasetExperiment object
name	DatasetExperiment slot to get/set
value	the value to assign to the named slot

Details

The DatasetExperiment object is an extension of the SummarizedExperiment object from the SummarizedExperiment package (found on Bioconductor). It incorporates the basic functionality of struct objects, containing fields such as Description, Name and Type with features of SummarizedExperiment such as subsetting.

There are some important differences between DatasetExperiment and SummarizedExperiment:

- In DatasetExperiment data is stored as Samples (rows) x Features (columns)
- DatasetExperiment currently only supports a single assay
- length(DatasetExperiment) returns the number of samples

Value

DatasetExperiment

Slots

name Name of the dataset

description Brief description of the dataset

type The type of dataset e.g. single_block

---

entity_stato   *entity_stato class*

Description

A base class in the **struct** package. Should not be called directly.

Usage

```
entity_stato(
  name,
  description = character(0),
  type = "character",
  value = NULL,
  max_length = Inf,
  stato_id
)
```

Arguments

name	the name of the object
description	a description of the object
type	the type of the struct object
value	The value of the parameter/outputs
max_length	Maximum length of value vector (default 1)
stato_id	The STATO ID for the entity

Details

Extends the `entity` class to include stato functionality.

Value

an entity_stato object

See Also

Refer to entity and stato for further info.

Examples

```
E = entity_stato(
    name = 'example',
    description = 'this is an example',
    type = 'numeric',
    value = 1,
    stato_id='XYZ000001'
)
```

---

enum *Enum objects*

Description

A base class in the **struct** package. Not normally called directly.

Usage

```
enum(
  name,
  description = character(0),
  type = "character",
  value = character(0),
  max_length = 1,
  allowed,
  ...
)

## S4 replacement method for signature 'enum'
value(obj) <- value
```

Arguments

name	the name of the object
description	a description of the object
type	the type of the struct object
value	value of the enum
max_length	Maximum length of value vector (default 1)
allowed	A list of allowed values
...	additional inputs to the struct_class object
obj	an enum object

Details

An enum object is a special type of entity object that ensures the value must be one from a list of allowed values.

Enum objects are usually defined in the prototype of another object, but can be extracted using `param_obj` and `output_obj`.

Value

an enum object

Examples

```
# Create a new enum object
E = enum(
    name = 'example',
    description = 'this is an example',
    type = 'character',
    value = 'hello',
    allowed = c('hello','world')
)

# Get/set the value of the entity object
value(E)
value(E) = 'world'
```

---

enum_stato   *enum_stato class*

Description

A base class in the **struct** package. Should not be called directly.

Usage

```
enum_stato(
  name,
  description = character(0),
  type = "character",
  value = character(0),
  max_length = 1,
  allowed,
  stato_id
)
```

Arguments

name	the name of the object
description	a description of the object
type	the type of the struct object
value	The value of the parameter/outputs
max_length	Maximum length of value vector (default 1)
allowed	A list of allowed values
stato_id	The STATO ID for the entity

Details

Extends the enum class to include stato functionality.

Value

an enum_stato object

See Also

Refer to enum and stato for further info.

Examples

```
E = enum_stato(
    name='example',
    allowed=list('choice_1','choice_2'),
    value='choice_1',
    type='character',
    stato_id='XYZ000001'
)
```

---

example_chart   *example chart object*

Description

an example of a chart object for documentation purposes

Usage

```
example_chart(...)

## S4 method for signature 'example_chart,example_model'
chart_plot(obj, dobj)
```

Arguments

...	named slots and their values.
obj	a chart object
dobj	a example_model object

Value

a chart object

Examples

```
C = example_chart()
chart_plot(C,example_model())
```

```
example_iterator-class
```
Example iterator

Description

An example iterator for testing

runs the example iterator, which just returns a value of 3.142

Usage

```
## S4 method for signature 'example_iterator,DatasetExperiment,metric'
run(I, D, MET)
```

Arguments

I	example_iterator object
D	dataset object
MET	metric object

Value

test iterator object

dataset object

Examples

```
I = example_iterator()

I = example_iterator()
D = iris_DatasetExperiment()
MET = metric()
I = run(I,D,MET)
```

```
example_model
```
Example model

Description

An example model for testing. Training this model adds value_1 to a data set, and prediction using this model adds value_2.

trains the example model, which adds value_1 to the raw data of a dataset

predicts using the example model, which adds value_2 to the raw data of a dataset

Usage

```
example_model(value_0 = 0, value_1 = 10, value_2 = 20, ...)

## S4 method for signature 'example_model,DatasetExperiment'
model_train(M, D)

## S4 method for signature 'example_model,DatasetExperiment'
model_predict(M, D)
```

Arguments

value_0	a numeric value
value_1	a numeric value
value_2	a numeric value
...	named slots and their values.
M	A struct model object
D	A DatasetExperiment object

Value

modified example_model object

dataset object

dataset object

Examples

```
M = example_model()
M = example_model(value_1 = 10, value_2 = 20)
D = iris_DatasetExperiment()
M = example_model(value_1 = 10, value_2 = 20)
M = model_train(M,D)
D = iris_DatasetExperiment()
M = example_model(value_1 = 10, value_2 = 20)
M = model_predict(M,D)
```

---

export_xlsx   *write a dataset object to file*

Description

Exports a dataset object to an excel file with sheets for data, sample_meta and variable_meta

Usage

```
export_xlsx(object, outfile, transpose = TRUE)

## S4 method for signature 'DatasetExperiment'
export_xlsx(object, outfile, transpose = TRUE)
```

Arguments

object	a dataset object
outfile	the filename (including path) to write the data to
transpose	TRUE (default) or FALSE to transpose the output data

Value

an excel file with sheets for data and meta data

Examples

```
## Not run:
D = iris_DatasetExperiment() # example dataset
export_xlsx(D,'iris_DatasetExperiment.xlsx')

## End(Not run)
```

---

iris_DatasetExperiment

Fisher's Iris data

Description

Fisher's Iris data as a DatasetExperiment object

Usage

```
iris_DatasetExperiment()
```

Value

DatasetExperiment object

Examples

```
D = iris_DatasetExperiment()
```

`is_output`   *Verify output*

Description

Verify that the name of a output is valid for an object

Usage

```
is_output(obj, name)

## S4 method for signature 'struct_class'
is_output(obj, name)
```

Arguments

obj   A model or iterator object derived from the *struct* class

name   Name of output

Value

TRUE if output name is valid, FALSE if not

Methods (by class)

   • struct_class:

Examples

```
M = example_model()
is_output(M,'result_1') # TRUE
is_output(M,'result_0')  # FALSE
```

`is_param`   *Verify parameter*

Description

Verify that the input name is a valid input parameter for an object

Usage

```
is_param(obj, name)

## S4 method for signature 'struct_class'
is_param(obj, name)
```

Arguments

obj	An object derived from struct_class
name	Name of parameter

Value

TRUE if parameter name is valid, FALSE if not

Methods (by class)

- struct_class:

Examples

```
M = example_model()
is_param(M,'value_1') # TRUE
is_param(M,'alpha')   # FALSE
```

---

libraries	*Libraries for an object*

Description

All struct objects have a "libraries" slot, which is a character array of libraries required to use the object. The libraries method gathers libraries from an object and all struct objects that it inherits to generate a complete list.

Usage

```
libraries(obj)

## S4 method for signature 'struct_class'
libraries(obj)
```

Arguments

obj	a struct object

Value

a character array of R packages needed by the object

Examples

```
M = example_model()
libraries(M)
```

---

max_length   *get the max value vector length for an entity*

Description

A base class in the **struct** package. Not normally called directly. An entity object is used to store information about a parameter or output_ The standard 'name','description' and 'type' slots are included, along with 'value' for storing the value of the parameter and 'max_length' for restricting the length of 'value' if needed.

Usage

```
max_length(obj)

entity(
  name,
  description = character(0),
  type = "character",
  value = NULL,
  max_length = Inf,
  ...
)

## S4 method for signature 'entity'
value(obj)

## S4 replacement method for signature 'entity'
value(obj) <- value

## S4 method for signature 'entity'
max_length(obj)

## S4 replacement method for signature 'entity'
max_length(obj) <- value
```

Arguments

obj	An entity object
name	the name of the object
description	a description of the object
type	the type of the struct object
value	The value of the parameter/outputs
max_length	Maximum length of value vector (default 1)
...	additional inputs to the struct_class object

Details

Entity objects are usually defined in the prototype of another object, but can be extracted using `param_obj` and `output_obj`.

Value

max value vector length for an entity

An entity object

Examples

```
# Create a new entity object
E = entity(
    name = 'example',
    description = 'this is an example',
    type = 'numeric',
    value = 1
)

# Get/set the value of the entity object
value(E)
value(E) = 10
```

---

model *model class*

Description

A class for models that can be trained/applied to datasets e.g. PCA, PLS etc. Also used for preprocessing steps that require application to test sets. not intended to be called directly, this class should be inherited to provide functionality for method-specific classes.

Usage

```
model(
  predicted = character(0),
  seq_in = "data",
  seq_fcn = function(x) {     return(x) },
  ...
)

## S4 method for signature 'model,DatasetExperiment'
model_train(M, D)

## S4 method for signature 'model,DatasetExperiment'
model_predict(M, D)

## S4 method for signature 'model,DatasetExperiment'
```

```
model_apply(M, D)

## S4 method for signature 'model,DatasetExperiment'
model_reverse(M, D)

## S4 method for signature 'model'
predicted(M)

## S4 method for signature 'model'
seq_in(M)

## S4 replacement method for signature 'model,character'
seq_in(M) <- value

## S4 method for signature 'model'
predicted_name(M)

## S4 replacement method for signature 'model,character'
predicted_name(M) <- value
```

Arguments

predicted	The name of an output slot to return when using predicted() (see details)
seq_in	the name of an output slot to connect with the "predicted" output of another model (see details)
seq_fcn	a function to apply to seq_in before inputting into the next model. Typically used to extract a single column, or convert from factor to char etc.
...	named slots and their values.
M	A struct model object
D	A DatasetExperiment object
value	The value to assign

Value

trained model object

model object with test set results

trained model object

dataset dataset object with the reverse model applied

the predicted output, as specified by predicted_name

the id of the input parameter to be replaced by the predicted output of the previous model in a model sequence. Reserved keyword 'data' means that the input data used by model_train, model_apply etc is used. seq_in = 'data' is the default setting.

the modified model object

the id of the output returned by predicted()

the modified model object

predicted **slot**

The "predicted" slot is a slots for use by users to control the flow of model sequences. The predicted() function is used to return a default output and from a model. Typically it is a DatasetExperiment object that is passed directly into the next model in a sequence as the data for that model.

seq_in **slot**

In a sequence of models (see model_seq) the "predicted" slot is connected to the DatasetExperiment input of the next model. seq_in can be used to control flow and connect the "predicted" output to the input parameter of the next model. Default is the keyword 'data', and can otherwise be replaced by any input slot from the model. The slot seq_fcn can be used to apply a transformation to the output before it is used as an input. This allows you to e.g. convert between types, extract a single column from a data.frame etc.

Examples

```
M = model()
D = DatasetExperiment()
M = model()
M = model_train(M,D)
D = DatasetExperiment()
M = model()
M = model_train(M,D)
M = model_predict(M,D)
D = DatasetExperiment()
M = model()
M = model_apply(M,D)
D = DatasetExperiment()
M = model()
M = model_train(M,D)
M = model_predict(M,D)
M = model_reverse(M,D)
D = DatasetExperiment()
M = example_model()
M = model_train(M,D)
M = model_predict(M,D)
p = predicted(M)
D = DatasetExperiment()
M = example_model()
seq_in(M) = 'data'
M = example_model()
seq_in(M) = 'value_1'
M = example_model()
predicted_name(M)
M = example_model()
predicted_name(M) = 'result_2'
```

---

models   *Get/set models of a model_seq*

Description

Returns the list of models in a model_seq object

Usage

```
models(ML)

models(ML) <- value
```

Arguments

ML	a model_seq object
value	a list containing only model objects

Value

models(ML) returns a list of models in the model sequence

models(ML)<- sets the list of models in the model sequence

Examples

```
# Create a model sequence
ML = model_seq()
models(ML) = list(example_model(), example_model())
models(ML)
```

---

model_apply   *Apply a model*

Description

Applies a method to the input dataset

Usage

```
model_apply(M, D)
```

Arguments

M	a 'method' object
D	another object used by the first

Value

Returns a modified method object

Examples

```
M = example_model()
M = model_apply(M,iris_DatasetExperiment())
```

---

model_predict   *Model prediction*

Description

Apply a model using the input dataset. Assumes the model is trained first.

Usage

```
model_predict(M, D)
```

Arguments

M   a model object

D   a dataset object

Value

Returns a modified model object

Examples

```
M = example_model()
M = model_predict(M,iris_DatasetExperiment())
```

---

model_reverse   *Reverse preprocessing*

Description

Reverse the effect of a preprocessing step on a dataset_

Usage

```
model_reverse(M, D)
```

Arguments

M	a model object
D	a dataset object

Value

Returns a modified dataset object

Examples

```
M = example_model()
D = model_reverse(M,iris_DatasetExperiment())
```

---

model_seq   *model_seq class*

Description

A class for (ordered) lists of models

Usage

```
model_seq(...)

## S4 method for signature 'model_seq,DatasetExperiment'
model_train(M, D)

## S4 method for signature 'model_seq,DatasetExperiment'
model_predict(M, D)

## S4 method for signature 'model_seq,ANY,ANY,ANY'
x[i]

## S4 replacement method for signature 'model_seq,ANY,ANY,ANY'
x[i] <- value

## S4 method for signature 'model_seq'
models(ML)

## S4 replacement method for signature 'model_seq,list'
models(ML) <- value

## S4 method for signature 'model_seq'
length(x)

## S4 method for signature 'model,model_seq'
e1 + e2
```

```
## S4 method for signature 'model_seq,model'
e1 + e2

## S4 method for signature 'model,model'
e1 + e2

## S4 method for signature 'model_seq'
predicted(M)

## S4 method for signature 'model_seq,DatasetExperiment'
model_apply(M, D)
```

Arguments

...	named slots and their values.
M	a model object
D	a dataset object
x	a model_seq object
i	index
value	value
ML	a model_seq object
e1	a model or model_seq object
e2	a model or model_seq object

Value

model sequence

model sequence

model at the given index in the sequence

model sequence with the model at index i replaced

a list of models in the sequence

a model sequence containing the input models

the number of models in the sequence

a model sequence with the additional model appended to the front of the sequence

a model sequence with the additional model appended to the end of the sequence

a model sequence

the predicted output of the last model in the sequence

Examples

```
MS = model_seq()
MS = model() + model()
MS = example_model() + example_model()
MS = model_train(MS,DatasetExperiment())
D = DatasetExperiment()
MS = example_model() + example_model()
MS = model_train(MS,D)
MS = model_predict(MS,D)
MS = model() + model()
MS[2]

MS = model() + model()
MS[3] = model()

MS = model() + model()
L = models(MS)

MS = model_seq()
L = list(model(),model())
models(MS) = L

MS = model() + model()
length(MS) # 2

MS = model() + model()
M = model()
MS = M + MS

MS = model() + model()
M = model()
MS = MS + M

MS = model() + model()

D = DatasetExperiment()
M = example_model()
M = model_train(M,D)
M = model_predict(M,D)
p = predicted(M)
D = DatasetExperiment()
MS = example_model() + example_model()
MS = model_apply(MS,D)
```

---

model_train   *Train a model*

Description

Trains a model using the input dataset

Usage

```
model_train(M, D)
```

Arguments

M	a model object
D	a dataset object

Value

Returns a modified model object

Examples

```
M = example_model()
M = model_train(M,iris_DatasetExperiment())
```

---

new_struct	*Generate a* **struct** *object from a Class*

Description

This function creates a newly allocated object from the class identified by the first argument. It works almost identically to `new` but is specific to objects from the **struct** package and ensures that `entity` slots have their values assigned correctly. This function is usually called by class constructors and not used directly.

Usage

```
new_struct(class, ...)
```

Arguments

class	The class of struct object to create
...	named slots and values to assign

Value

An object derived from struct_class

Examples

```
S = new_struct('struct_class')
```

---

ontology   *Ontology for an object*

Description

All `struct` objects have an "ontology" slot, which is a list of ontology items for the object. The `ontology` method gathers ontology items from an object and all `struct` objects that it inherits to generate a complete list.

A base class in the **struct** package. Stores ontology information e.g. term, description, id etc for struct objects and provides methods for populating these fields using the 'rols' package.

A base class in the **struct** package. Stores multiple 'ontology_term' objects.

Usage

```
ontology(obj, cache = NULL)

ontology_term(
  id,
  ontology = character(),
  label = character(),
  description = character(),
  iri = character(),
  rols = TRUE
)

ontology_list(terms = list())

## S4 method for signature 'ontology_list,ANY,ANY,ANY'
x[i]

## S4 replacement method for signature 'ontology_list,ANY,ANY,ANY'
x[i] <- value

## S4 method for signature 'ontology_list'
length(x)

## S4 method for signature 'struct_class'
ontology(obj, cache = NULL)
```

Arguments

obj	a struct object
cache	a named list of ontology_terms for offline use. Terms from the cache are search based on the name of the list items matching the ontology id. If cache=NULL then the OLS API is used to lookup terms.
id	(character) The ontology term id e.g. 'STATO:0000555'

ontology	(character) The ontology the term is a member of e.g. 'stato'
label	(character) The label for the ontology term
description	(character) The description of the term
iri	(character) The Internationalized Resource Identifier for the term
rols	(logical) TRUE or FALSE to query the Ontology Lookup Service for missing label, description or iri if not provided as input. Default rols = TRUE
terms	A list of ontology_term objects.
x	the list
i	The list item index
value	an ontology_term() object

Value

model at the given index in the sequence

model sequence with the model at index i replaced

the number of models in the sequence

Examples

```
M = example_model()
ontology(M,cache=NULL)
## Not run:
OT = ontology_term(id='STATO:0000555')

## End(Not run)
## Not run:
OT = ontology_list(terms=list(
    ontology_term(ontology='obi',id =  'OBI:0200051'),
    ontology_term(ontology='stato',id ='STATO:0000555')
)

## End(Not run)
## Not run:
OL = ontology_list('STATO:0000555')
OL[1]

## End(Not run)

## Not run:
OL = ontology_list('STATO:0000555')
OL[1] = ontology_term('STATO:0000302')

## End(Not run)
## Not run:
OL = ontology_list()
length(OL) # 0

## End(Not run)
```

---

optimiser	*optimiser class*

Description

A special class of iterator for selecting optimal parameter values not intended to be called directly, this class should be inherited to provide functionality for method-specific classes.

Usage

```
optimiser(...)
```

Arguments

...	named slots and their values.

Value

an optimiser object

Examples

```
OPT = optimiser()
```

---

output_ids	*Output identifiers*

Description

return a list of valid output ids for an object

Usage

```
output_ids(obj)

## S4 method for signature 'struct_class'
output_ids(obj)
```

Arguments

obj	A model or iterator object derived from the *struct* class

Value

list of output ids

Methods (by class)

- struct_class:

Examples

```
M = example_model()
output_ids(M)
```

---

output_list	*output list*

Description

get/set a named list of outputs and their current value for an object

Usage

```
output_list(obj)

output_list(obj) <- value

## S4 method for signature 'struct_class'
output_list(obj)

## S4 replacement method for signature 'struct_class,list'
output_list(obj) <- value
```

Arguments

obj	An object derived from struct_class
value	A named list of outputs and corresponding values

Value

A named list of outputs and corresponding values

struct object

Methods (by class)

- struct_class:
- obj = struct_class, value = list:

Examples

```
M = example_model()
L = output_list(M)
M = example_model()
output_list(M) = list('result_1' = DatasetExperiment(),'result_2' = DatasetExperiment())
```

---

output_name   *output name*

Description

return a the name for a output, if available

Usage

```
output_name(obj, name)

## S4 method for signature 'struct_class,character'
output_name(obj, name)
```

Arguments

obj   A model or iterator object derived from the *struct* class

name   Name of output

Value

name of output

Methods (by class)

- obj = struct_class, name = character:

Examples

```
M = example_model()
output_name(M,'result_1')
```

---

output_obj   *Output objects*

Description

Gets or sets the object of an output e.g. to an entity() object.

Usage

```
output_obj(obj, name)

output_obj(obj, name) <- value

## S4 method for signature 'struct_class,character'
output_obj(obj, name)

## S4 replacement method for signature 'struct_class,character'
output_obj(obj, name) <- value
```

Arguments

obj	A model or iterator object derived from the *struct* class
name	Name of output
value	A valid value for the output being set

Value

`output_obj(M,name)` returns the named output as an object

`output_obj(M,name)<-` sets the named output of an object

the modified object

Methods (by class)

- `obj = struct_class,name = character`:
- `obj = struct_class,name = character`:

Examples

```
# get the output as an object
M = example_model()
obj = output_obj(M, 'result_1')

# set a output as an object
output_obj(M, 'result_1') = entity(value = 15,type = 'numeric',name = 'result_1')
```

---

output_value   *output values*

Description

get/set the values for an output_

Usage

```
output_value(obj, name)

output_value(obj, name) <- value

## S4 method for signature 'struct_class,character'
output_value(obj, name)

## S4 replacement method for signature 'struct_class,character'
output_value(obj, name) <- value
```

Arguments

obj	A model or iterator object derived from the *struct* class
name	Name of output
value	A valid value for the output being set

Value

Value of output

struct object

Methods (by class)

- obj = `struct_class`,name = `character`:
- obj = `struct_class`,name = `character`:

Examples

```
M = example_model()
output_value(M,'result_1')
M = example_model()
output_value(M,'result_1') = DatasetExperiment()
```

---

param_ids *Parameter identifiers*

Description

return a list of valid parameter ids for an object

Usage

```
param_ids(obj)

## S4 method for signature 'struct_class'
param_ids(obj)
```

Arguments

obj   An object derived from struct_class

Value

list of parameter ids

Methods (by class)

- struct_class:

Examples

```
M = example_model()
param_ids(M)
```

---

param_list   *Parameter list*

Description

get/set a named list of parameters and thier current value for an object

Usage

```
param_list(obj)

param_list(obj) <- value

## S4 method for signature 'struct_class'
param_list(obj)

## S4 replacement method for signature 'struct_class,list'
param_list(obj) <- value
```

Arguments

obj   An object derived from struct_class

value   A named list of parameters and corresponding values

Value

A named list of parameters names and corresponding values

Methods (by class)

- struct_class:
- obj = struct_class, value = list:

Examples

```
M = example_model()
L = param_list(M)

M = example_model()
param_list(M) = list('value_1' = 15,'value_2' = 20)
```

---

param_name   *Parameter name*

Description

Returns the name for a parameter, if available

Usage

```
param_name(obj, name)

## S4 method for signature 'struct_class,character'
param_name(obj, name)
```

Arguments

obj	An object derived from struct_class
name	Name of parameter

Value

name of parameter

Methods (by class)

- obj = struct_class,name = character:

Examples

```
M = example_model()
param_name(M,'value_1')
```

---

param_obj   *Parameter objects*

Description

Gets or sets the object of a parameter e.g. to an entity() object.

Usage

```
param_obj(obj, name)

param_obj(obj, name) <- value

## S4 replacement method for signature 'struct_class,character'
param_obj(obj, name) <- value

## S4 method for signature 'struct_class,character'
param_obj(obj, name)
```

Arguments

obj   An object derived from struct_class

name   Name of parameter

value   A valid value for the parameter being set

Value

`param_obj(M,name)` Returns the named parameter as an object

`param_obj(M,name)<-` Sets the named parameter of an object

Examples

```
# get the parameter as an object
M = example_model()
obj = param_obj(M, 'value_0')

# set a parameter as an object
param_obj(M, 'value_0') = entity(value = 15,type = 'numeric',name='value_0')
```

---

param_value   *Parameter values*

Description

get/set the values for a parameter.

Usage

```
param_value(obj, name)

param_value(obj, name) <- value

## S4 method for signature 'struct_class,character'
param_value(obj, name)

## S4 replacement method for signature 'struct_class,character'
param_value(obj, name) <- value
```

Arguments

obj	A model or iterator object derived from structclass
name	Name of parameter
value	A valid value for the parameter being set

Value

Value of parameter

Methods (by class)

- `obj = struct_class,name = character`:
- `obj = struct_class,name = character`:

Examples

```
M = example_model()
param_value(M,'value_1')

M = example_model()
param_value(M,'value_1') = 0.95
```

---

predicted *Prediction output*

Description

returns the prediction output for a model_ This is supplied as input to the next model when used in a model_seq

Usage

```
predicted(M)
```

Arguments

M   a model object

Value

The value returned varies depending on the output_

Examples

```
M = example_model()
M = model_train(M, iris_DatasetExperiment())
M = model_predict(M, iris_DatasetExperiment())
predicted(M)
```

---

predicted_name *Predicted output name*

Description

get/set the prediction output for a model_ This determines which outputs from this model are supplied as inputs to the next model when used in a model_seq

Usage

```
predicted_name(M)

predicted_name(M) <- value
```

Arguments

M   a model object

value   name of an output for this model

Value

predicted_name returns the name of the predicted output

predicted_name<- sets the name of the predicted output

Examples

```
M = example_model()
predicted_name(M)
predicted_name(M) = 'result_2'
```

---

preprocess   *preprocessing class*

Description

A class used for preprocessing steps that require application to test sets. not intended to be called directly, this class should be inherited to provide functionality for method-specific classes.

Usage

```
preprocess(...)

## S4 method for signature 'preprocess,DatasetExperiment'
model_reverse(M, D)
```

Arguments

...	named slots and their values.
M	a model object
D	a dataset object

Value

dataset object

Examples

```
M = preprocess()
D = DatasetExperiment()
M = model()
D2 = model_reverse(M,D)
```

---

resampler *resampler class*

Description

A class for resampling methods such as cross-validation. not intended to be called directly.

Usage

```
resampler(...)
```

Arguments

`...` named slots and their values.

Value

a resampler object

Examples

```
R = resampler()
```

---

result *Iterator result*

Description

Returns the results of an iterator. This is used to control model flow in a similar way to `predict` for model and model_seq objects.

Usage

```
result(M)
```

Arguments

`M` an iterator object

Value

the returned output varies with the algorithm implemented

Examples

```
D = iris_DatasetExperiment() # get some data
MET = metric()  # use a metric
I = example_iterator() # initialise iterator
models(I) = example_model() # set the model
I = run(I,D,MET) # run
result(I)
```

---

result_name   *get/set output name as prediction output for a model*

Description

get/set the prediction output for a model_ This determines which outputs from this model are supplied as inputs to the next model when used in a model_seq

Usage

```
result_name(M)

result_name(I) <- value
```

Arguments

M	an iterator object
I	an iterator object
value	name of an output for iterator M

Value

result_name(M) returns the name of the output for this iterator (equivalent to `predicted` for model objects)

result_name(I)<- sets the default output for an iterator

Examples

```
I = example_iterator() # initialise iterator
result_name(I)
result_name(I) = 'result_1'
```

run   *Run iterator*

Description

Runs an iterator, applying the chosen model multiple times.

Evaluates an iterator by e.g. averaging over all iterations. May be deprecated in a future release as `evaluate` is applied by `run` anyway.

A class for iterative approaches that involve the training/prediction of a model multiple times. Not intended to be called directly, this class should be inherited to provide functionality for method-specific classes.

Usage

```
run(I, D, MET)

evaluate(I, MET)

iterator(...)

## S4 method for signature 'iterator,DatasetExperiment,metric'
run(I, D, MET = NULL)

## S4 method for signature 'iterator,metric'
evaluate(I, MET)

## S4 method for signature 'iterator'
models(ML)

## S4 replacement method for signature 'iterator,model_OR_iterator'
models(ML) <- value

## S4 replacement method for signature 'iterator,character'
result_name(I) <- value

## S4 method for signature 'iterator'
result(M)

## S4 method for signature 'iterator'
result_name(M)

## S4 method for signature 'iterator,model_OR_iterator'
e1 * e2

## S4 method for signature 'iterator,ANY,ANY,ANY'
x[i]
```

```
## S4 replacement method for signature 'iterator,ANY,ANY,ANY'
x[i] <- value
```

Arguments

I	an iterator object
D	a dataset object
MET	a metric object
...	named slots and their values.
ML	a model sequence object
value	value
M	a model object
e1	an iterator object
e2	an iterator or a model object
x	a sequence object
i	index into sequence

Details

Running an iterator will apply the iterator a number of times to a dataset_ For example, in cross-validation the same model is applied multiple times to the same data, splitting it into training and test sets. The input metric object can be calculated and collected for each iteration as an output_

Value

Modified iterator object

Modified iterator object

the modified model object

model at the given index in the sequence

iterator with the model at index i replaced

Examples

```
D = iris_DatasetExperiment() # get some data
MET = metric()  # use a metric
I = example_iterator() # initialise iterator
models(I) = example_model() # set the model
I = run(I,D,MET) # run
D = iris_DatasetExperiment() # get some data
MET = metric()  # use a metric
I = example_iterator() # initialise iterator
models(I) = example_model() # set the model
I = run(I,D,MET) # run
I = evaluate(I,MET) # evaluate
I = iterator()
```

```
I = iterator() * model()
D = DatasetExperiment()
MET = metric()
I = iterator() * model()
I = run(I,D,MET)

I = iterator()
result_name(I) = 'example'
MS = model() + model()
I = iterator() * MS
I[2] # returns the second model() object

MS = model() + model()
I = iterator() * MS
I[2] = model() # sets the second model to model()
```

---

seq_in   *Sequence input*

Description

get/set the input parameter replaced by the output of the previous model in a model sequence. Default is "data" which passes the output as the data input for methods such as `model_train` and `model_apply`.

Usage

```
seq_in(M)

seq_in(M) <- value
```

Arguments

M	a model object
value	name of an output for this model

Value

`seq_in` returns the name of the input parameter replaced when used in a model sequence

`seq_in<-` sets the name of the input parameter replaced when used in a model sequence

Examples

```
M = example_model()
seq_in(M)
seq_in(M) = 'value_1'
```

| set_obj_method | *update method for a struct object* |

Description

a helper function to update methods for a struct object

Usage

```
set_obj_method(
  class_name,
  method_name,
  definition,
  where = topenv(parent.frame()),
  signature = c(class_name, "DatasetExperiment")
)
```

Arguments

class_name	the name of the to update the method for
method_name	the name of the method to update. Must be an existing method for the object.
definition	the function to replace the method with. This function will be used when the method is called on the object.
where	the environment to create the object in. default where = topenv(parent.frame())
signature	a list of classes that this object requires as inputs. Default is c(class_name,'DatasetExperiment')

Value

a method is created in the specified environment

Examples

```
set_struct_obj(
class_name = 'add_two_inputs',
struct_obj = 'model',
params = c(input_1 = 'numeric', input_2 = 'numeric'),
outputs = c(result = 'numeric'),
prototype = list(
   input_1 = 0,
   input_2 = 0,
   name = 'Add two inputs',
   description = 'example class that adds two values together')
)
```

---

set_obj_show *a helper function to update the show method for a struct object*

Description

a helper function to update the show method for a struct object

Usage

```
set_obj_show(class_name, extra_string, where = topenv(parent.frame()))
```

Arguments

`class_name`	the name of the to update the method for
`extra_string`	a function that returns an extra string using the input object as an input e.g. function(object)return = 'extra_string'
`where`	the environment to create the object in. default where = topenv(parent.frame())

Value

a method is created in the specified environment

Examples

```
# create an example object first
set_struct_obj(
class_name = 'add_two_inputs',
struct_obj = 'model',
params = c(input_1 = 'numeric', input_2 = 'numeric'),
outputs = c(result = 'numeric'),
prototype = list(
   input_1 = 0,
   input_2 = 0,
   name = 'Add two inputs',
   description = 'example class that adds two values together')
)

# now update the method
set_obj_show(
class_name = 'add_two_inputs',
extra_string = function(object) {return('The extra text')}
)
```

---

set_struct_obj *define a new struct object*

Description

a helper function to create new struct objects

Usage

```
set_struct_obj(
  class_name,
  struct_obj,
  params = character(0),
  outputs = character(0),
  private = character(0),
  prototype = list()
)
```

Arguments

class_name	the name of the new class to create
struct_obj	the struct obj to inherit e.g. 'model', 'metric' etc
params	a named character vector of input parameters where each element specifies the type of value that will be in the slot e.g. c(example = 'character')
outputs	a named character vector of outputs where each element specifies the type of value that will be in the slot e.g. c(example = 'character')
private	a named character vector of private slots where each element specifies the type of value that will be in the slot e.g. c(example = 'character'). These are intended for internal use by the object and generally not available to the user.
prototype	a named list with initial values for slots.

Value

a new class definition. to create a new object from this class use X = new_class_name()

---

stato_id *get the stato_id for an object*

Description

A base class in the **struct** package. Provides several fundamental methods and should not be called directly.

Usage

```
stato_id(obj)

stato_name(obj)

stato_definition(obj)

stato_summary(obj)

stato(stato_id)

## S4 method for signature 'stato'
stato_id(obj)

## S4 method for signature 'stato'
stato_name(obj)

## S4 method for signature 'stato'
stato_definition(obj)

## S4 method for signature 'stato'
stato_summary(obj)
```

Arguments

obj	An object derived from the stato object
stato_id	A STATO ID e.g. OBI:0000001

Details

STATO is the statistical methods ontology. It contains concepts and properties related to statistical methods, probability distributions and other concepts related to statistical analysis, including relationships to study designs and plots (see http://stato-ontology.org/).

This class provides access to a version of the STATO ontology database that can be searched by ontology id to provide formal names and definitions for methods, models, iterators, metrics and charts.

This class makes use of the `ontologyIndex` package to search a copy of the STATO database included in this package.

Value

id the stato id

name the stato name

def the stato description

Value returned depends on the method used.

Examples

```
M = example_model()
stato_id(M)
stato_name(M)
stato_definition(M)
stato_summary(M)
# an example stato object
M = example_model()

# the stato id assigned to object M
stato_id(M) # OBI:0000011

# the name associated with that id
stato_name(M)

# the STATO definition for that id
stato_definition(M)

# a summary of the STATO database entry for the id, and any parameters or
# outputs that also have stato ids.
stato_summary(M)
```

---

struct   *StRUCT: Statistics in R Using Class Templates*

Description

This package defines classes (templates) for developing statistical workflows. These classes can be extended using other packages, making it easier to combine methods from different packages into a robust workflow. Integration with STATO: the statistical methods ontology (`https://www.ebi.ac.uk/ols/ontologies/stato`) provides standardised definitions for many statistical methods.

Classes

The classes include:

- **DatasetExperiment**: An extension of the SummarizedExperiment object by Bioconductor

- **model**: A template for training and applying statistics

- **iterator**: A template for resampling, optimisation and validation of statistical models

- **chart**: A template for generating graphical outputs for models and iterators

---

struct_class *Constructor for struct_class objects*

Description

Creates a new struct_class object and populates the slots. Not intended for direct use.

Usage

```
struct_class(
  name = character(0),
  description = character(0),
  type = character(0),
  citations = list(),
  ontology = character(0)
)
```

Arguments

name	the name of the object
description	a description of the object
type	the type of the struct object
citations	a list of citations for the object in "bibentry" format
ontology	a list of ontology items for the object in "ontology_item" format

Value

a struct_class object

---

struct_class-class struct_class *object definition*

Description

Defines the struct class base template. This class is inherited by other objects and not intended for direct use. It defines slots and methods common to all **struct** objects.

Value

Returns a **struct** object

Public slots

Public slots can be accessed using shorthand $ notation and are intended for users building workflows.

name character() A short descriptive name of the struct object

description character() A longer description of the struct object and what it does

type character() A keyword that describes the type of struct object

libraries character() A (read only) list of R packages used by this struct object

citations list of bibentry A (read only) list of citations relevant to this struct object, in Bibtex format.

Private slots

Private slots are not readily accessible to users and are intended for developers creating their own struct objects. Any slot not listed within '.params' or '.outputs' is considered a private slot.

.params character() A list of additional slot names that can be get/set by the user for a specific struct object. These are used as input parameters for different methods.

.outputs character() a list of additional slot names that can be get by the user. These are used to store the results of a method.

Examples

```
S = struct_class(name = 'Example',description = 'An example object')
```

---

struct_template   *StRUCT templates*

Description

Create a struct template

Usage

```
struct_template(
  template = "model",
  output,
  in_editor = TRUE,
  overwrite = FALSE
)
```

Arguments

template	the type of object you want a template for e.g. 'model'
output	the name/path of the output file
in_editor	TRUE/FALSE to open the created file in the default editor
overwrite	= TRUE/FALSE to overwrite file if exists already

Value

A template is created at the output location specified

Examples

```
## Not run:
struct_template('model','example.R',FALSE)

## End(Not run)
```

test_metric-class   *Example metric*

Description

An example metric for testing

calculates a metric, which just returns a value of 3.142

Usage

```
## S4 method for signature 'test_metric'
calculate(obj)
```

Arguments

obj   metric object

Value

test metric object

dataset object

Examples

```
MET = test_metric()

MET = test_metric()
MET = calculate(MET)
```

`$,ontology_list-method`

Get/set ontology_list slots

Description

Dollar syntax can be used to as a shortcut for getting values for ontology_list objects.

Usage

```
## S4 method for signature 'ontology_list'
x$name
```

Arguments

x   An ontology_term object

name   The name of the slot to access

Value

Slot value

Examples

```
## Not run:
OL = ontology_list('STATO:0000555')
OL$terms

## End(Not run)
```

`$,ontology_term-method`

Get/set ontology term slots

Description

Dollar syntax can be used to as a shortcut for getting values for ontology_term objects.

Usage

```
## S4 method for signature 'ontology_term'
x$name
```

Arguments

x   An ontology_term object

name   The name of the slot to access

Value

Slot value

Examples

```
## Not run:
OT = ontology_term(ontology='stato',id='STATO:0000555')

## End(Not run)
```

`$,struct_class-method` *Get/set parameter or output values*

Description

Dollar syntax can be used to as a shortcut for getting/setting input parameter and output values for struct objects.

Usage

```
## S4 method for signature 'struct_class'
x$name
```

Arguments

x   An object derived from struct_class

name   The name of the slot to access

Value

Parameter/output value

Examples

```
M = example_model()
M$value_1 = 10
M$value_1 # 10
```

$<-,struct_class-method

Get/set parameter or output values

Description

Dollar syntax can be used to as a shortcut for getting/setting input parameter and output values for struct objects.

Usage

```
## S4 replacement method for signature 'struct_class'
x$name <- value
```

Arguments

x	An object derived from struct_class
name	The name of the slot to access
value	The value to assign

Value

Parameter/output value

Examples

```
M = example_model()
M$value_1 = 10
M$value_1 # 10
```

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