Package 'nonmemica'

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Type Package

Title Create and Evaluate NONMEM Models in a Project Context					
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Maintainer Tim Bergsma dergsmat@gmail.com>					
Description Systematically creates and modifies NONMEM(R) control streams. Harvests NONMEM output, builds run logs, creates derivative data, generates diagnostics. NONMEM (ICON Development Solutions https://www.iconplc.com/) is software for nonlinear mixed effects modeling. See 'package?nonmemica'.					
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Description

Checks if file path is absolute.

Usage

absolute(x)

Arguments

x character (a file path)

Value

```
logical; TRUE if x starts with / or .: (e.g. C:)
```

as.best.default

Convert Vector to Best of Numeric or Character

Description

Convert vector to best of numeric or character.

Usage

```
## Default S3 method:
as.best(x, prefix = "", na.strings = c(".", "NA", ""), ...)
```

Arguments

```
x default
prefix prefix for viewing numerics
na.strings strings that should be treated as NA
... ignored
```

Details

Converts vector to numeric if doing so creates no new NA; otherwise to character. Number-like vectors that are nevertheless character are prefixed by default to make this explicit when viewing only a few rows.

See Also

```
Other util: %contains%(), as.best(), enclose(), locf(), padded(), parens(), pool(), runhead(), text2decimal()
```

```
as.bootstrap.bootstrap
```

Create Bootstrap from Bootstrap

Description

Creates bootstrap from bootstrap.

Usage

```
## S3 method for class 'bootstrap'
as.bootstrap(x, ...)
```

as.halfmatrix.default 5

Arguments

```
x bootstrap
... ignored
```

Value

data.frame

See Also

```
Other as.bootstrap: as.bootstrap(), as.bootstrap.numeric()
```

```
as.halfmatrix.default Coerce to Half Matrix by Default
```

Description

Coerces to half matrix. Treats x as halfmatrix, coerces to matrix and takes half.

Usage

```
## Default S3 method:
as.halfmatrix(x, ...)
```

Arguments

- x object
- ... passed arguments

```
Other halfmatrix: as.data.frame.halfmatrix(), as.halfmatrix(), as.halfmatrix.halfmatrix(), as.matrix.halfmatrix(), half(), half.matrix(), is.square(), is.square.matrix(), offdiag(), offdiag.halfmatrix(), ord.halfmatrix(), ord.matrix(), print.halfmatrix()
```

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as.init.init

Coerce init to init

Description

Coerces init to init

Usage

```
## S3 method for class 'init'
as.init(x = numeric(0), fixed = FALSE, comment = character(0), ...)
```

Arguments

x init
fixed logical
comment character

... passed arguments

Value

init

See Also

```
Other as.init: as.init(), as.init.numeric()
```

as.inits.list

Coerce list to inits

Description

Coerces list to inits.

Usage

```
## S3 method for class 'list'
as.inits(x, comment = character(0), ...)
```

Arguments

x list comment character

... passed arguments

as.matrix.halfmatrix 7

Value

inits

See Also

```
Other as.inits: as.inits(), as.inits.numeric()
```

```
as.matrix.halfmatrix Coerce Half Matrix to Matrix
```

Description

Coerces half matrix to matrix.

Usage

```
## S3 method for class 'halfmatrix' as.matrix(x, ...)
```

Arguments

```
x object ... passed arguments
```

See Also

```
Other halfmatrix: as.data.frame.halfmatrix(), as.halfmatrix(), as.halfmatrix.default(), as.halfmatrix.halfmatrix(), half(), half.matrix(), is.square(), is.square.matrix(), offdiag(), offdiag.halfmatrix(), ord.halfmatrix(), ord.matrix(), print.halfmatrix()
```

as.model.character

Coerce character to model

Description

Coerces chacter to model.

Usage

```
## S3 method for class 'character'
as.model(
    x,
    pattern = "^\\s*\\$(\\S+)(\\s.*)?$",
    head = "\\1",
    tail = "\\2",
    parse = TRUE,
    ...
)
```

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Arguments

x character

pattern pattern to identify record declarations head subpattern to identify declaration type

tail subpattern remaining

parse whether to convert thetas omegas and sigmas to inits, tables to items, and run-

records to fields

... ignored

Value

list

See Also

```
Other as.model: [.model(), [[.model(), as.model.numeric(), read.model(), write.model()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model
```

as.xml_document

Create an xml_document in a Project Context

Description

Creates an xml_document in a project context.

Coerces xml_document to xml_document

Usage

```
as.xml_document(x, ...)
## S3 method for class 'xml_document'
as.xml_document(x, ...)
```

Arguments

```
x xml_document
```

... ignored

Value

```
xml_document xml_document
```

Methods (by class)

• as.xml_document(xml_document): xml_document method

See Also

```
xpath
Other xpath: as.xml_document.character(), as.xml_document.numeric(), xpath(), xpath.default(),
xpath.xml_document()
Other xpath: as.xml_document.character(), as.xml_document.numeric(), xpath(), xpath.default(),
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.xml_document
```

```
as.xml_document.character
```

xpath.xml_document()

Create xml_document From Character

Description

Creates an xml_document from character (modelname or filepath).

Usage

```
## S3 method for class 'character'
as.xml_document(x, strip.namespace = TRUE, ...)
```

Arguments

```
x file path or run name
strip.namespace
whether to strip e.g. nm: from xml elements
... passed to modelpath()
```

Value

```
xml_document
```

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See Also

```
Other xpath: as.xml_document(), as.xml_document.numeric(), xpath(), xpath.default(),
xpath.xml_document()
```

as_nms_canonical

Coerce to 'nms_canonical'

Description

Coerces character to 'nms_canonical'.

ignored

Usage

```
as_nms_canonical(x, ...)
```

Arguments

x character

See Also

Other nms: as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()

as_nms_nonmem

Coerce to 'nms_nonmem'

Description

Coerces character to 'nms_nonmem'.

Usage

```
as_nms_nonmem(x, ...)
```

Arguments

x character

... ignored

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See Also

Other nms: as_nms_canonical(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()

as_nms_pmx

Coerce to 'nms_pmx'

Description

Coerces character to 'nms_pmx'.

Usage

```
as_nms_pmx(x, ...)
```

Arguments

x character ... ignored

See Also

Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()

as_nms_psn

Coerce to 'nms_psn'

Description

Coerces character to 'nms_psn'.

Usage

```
as_nms_psn(x, ...)
```

Arguments

x character ... ignored

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See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

comments.inits

Extract Comments from Inits

Description

Extracts comments from inits.

Usage

```
## S3 method for class 'inits'
comments(x, type, prior, ...)
```

Arguments

```
    x inits
    type item type: theta, omega, sigma (tables give items not inits)
    prior number of prior items of this type (maybe imporant for numbering)
    ignored
```

Value

data.frame

```
Other comments: comments(), comments.items(), comments.model()
```

comments.items 13

comments.items

Extract Comments from Items

Description

Extracts comments from items.

Usage

```
## S3 method for class 'items'
comments(x, ...)
```

Arguments

```
x items
... ignored
```

Value

data.frame

See Also

```
Other comments: comments(), comments.inits(), comments.model()
```

comments.model

Extract Comments from Model

Description

Extracts comments from model.

Usage

```
## S3 method for class 'model'
comments(
    x,
    fields = c("symbol", "unit", "label"),
    expected = character(0),
    na = NA_character_,
    tables = TRUE,
    ...
)
```

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Arguments

x model

fields data items to scavenge from control stream comments

expected parameters known from NONMEM output

na string to use for NA values when writing default metafile

tables whether to include table comments

... passed arguments

Value

data.frame

See Also

```
Other comments: comments(), comments.inits(), comments.items()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% comments
```

contains

Check Whether Text Contains Pattern

Description

Checks whether text contains pattern.

Usage

```
contains(pattern, text, ...)
```

Arguments

pattern regular expression
text character vector to check
... arguments to methods

Value

logical

See Also

%contains%

datafile.character 15

datafile.character

Identify the Datafile for a Model

Description

Identifies the datafile used by a model. Expresses it relative to current working directory.

Usage

```
## S3 method for class 'character' datafile(x, \ldots)
```

Arguments

x the model name or path to a control stream

... ext can be passed to modelfile, etc.

Value

character

See Also

```
Other path: datafile(), datafile.numeric(), modeldir(), modelfile(), modelpath(), modelpath.character(), modelpath.numeric(), psn_options(), specfile(), specfile.character(), specfile.numeric()
```

Examples

```
library(spec)
source <- system.file(package = 'nonmemica','project')
target <- tempdir()
target <- gsub('\\\','/',target) # for windows
file.copy(source,target,recursive = TRUE)
project <- file.path(target,'project','model')
options(project = project)
library(magrittr)
1001 %>% datafile
datafile(1001) %matches% specfile(1001)
1001 %>% specfile
1001 %>% specfile %>% read.spec
```

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definitions

Harvest Model Item Definitions

Description

Havests model item definitions.

Create Item Definitions from Model Name

Usage

```
definitions(x, ...)
## S3 method for class 'character'
definitions(
    x,
    verbose = FALSE,
    ctlfile = modelfile(x, ...),
    metafile = modelpath(x, "def", ...),
    fields = getOption("fields", default = c("symbol", "label", "unit")),
    read = length(metafile) == 1,
    write = FALSE,
    ...
)
```

Arguments

```
x object of dispatch
... arguments to methods

verbose set FALSE to suppress messages

ctlfile path to control stream (pass length-zero argument to ignore)

metafile path to definitions file (pass length-zero argument to ignore)

fields metadata fields to read from control stream if no metafile

read whether to read the definitions file

write whether to write the definitions file
```

Details

x can be numeric or character model name, assuming project is identified by argument or option.

Creates item definitions from a model name. Scavenges definitions optionally from the control stream and optionally from the definitions file. Optionally writes the result to the definitions file. Always returns a data.frame with at least the column 'item' but possibly no rows.

Value

object of class definitions, or path to metafile if write = TRUE.

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Methods (by class)

• definitions(character): character method

See Also

```
definitions.character
as.xml_document.character
as.bootstrap.character
as.model.character
Other definitions: definitions.definitions(), definitions.numeric()
Other definitions: definitions.definitions(), definitions.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% definitions
```

definitions.definitions

Create Model Item Definitions from definitions

Description

Creates a model item definitions from a definitions object.

Usage

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

Arguments

x definitions
... ignored

Details

Just returns the object unmodified.

```
Other definitions: definitions(), definitions.numeric()
```

18 errors.character

depends.default

Identify Model Dependencies

Description

Identify those models in the lineage of models in x.

Usage

```
## Default S3 method:
depends(x, ...)
```

Arguments

```
x object
```

... passed arguments

Value

character

See Also

Other depends: depends()

errors.character

Get Errors for Character

Description

Gets model asymptotic standard errors in canonical order, treating character as model names. See parameters for a less formal interface.

Usage

```
## S3 method for class 'character'
errors(
    x,
    xmlfile = modelpath(x, ext = "xml", ...),
    strip.namespace = TRUE,
    digits = 3,
    ...
)
```

estimates.character 19

Arguments

Value

numeric

See Also

```
nms_canonical errors
Other errors: errors(), errors.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% errors
```

estimates.character

Get Estimates for Character

Description

Gets model parameter estimates in canonical order, treating character as model names. See parameters for a less formal interface.

Usage

```
## S3 method for class 'character'
estimates(
    x,
    xmlfile = modelpath(x, ext = "xml", ...),
    strip.namespace = TRUE,
    digits = 3,
    ...
)
```

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Arguments

Value

numeric

See Also

```
nms_canonical errors
Other estimates: estimates(), estimates.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% estimates
```

fixed.init

Check if init is fixed

Description

Checks if init is fixed.

Usage

```
## S3 method for class 'init' fixed(x, ...)
```

Arguments

```
x init
... ignored
```

Value

logical

```
Other fixed: fixed(), fixed.model(), fixed<-(), fixed<-.init(), fixed<-.inits(), fixed<-.model()
```

fixed.model 21

fixed.model

Check If Model is Fixed

Description

Checks if model is fixed. Returns a logical vector with element for each init, in canonical order.

Usage

```
## S3 method for class 'model'
fixed(x, ...)
```

Arguments

x inits
... ignored

Value

logical

See Also

```
Other fixed: fixed(), fixed.init(), fixed<-.init(), fixed<-.inits(), fixed<-.model()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% fixed
```

generalize

Generalize a Nonmissing Value

Description

#Generalize a nonmissing value. If there is only one such among zero or more NA, impute that value for all NA.

Usage

```
generalize(x, ...)
```

Arguments

```
x vector ... ignored
```

22 ignored

See Also

```
Other superset: ignored(), meta(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

ignored

Extract Index for Ignored Records

Description

Extracts index for ignored records, given a NONMEM control stream.

Usage

```
ignored(
    x,
    read.input = list(read.csv, header = TRUE, as.is = TRUE),
    ext = getOption("modex", "ctl"),
    project = getOption("project", getwd()),
    nested = getOption("nested", TRUE),
    ...
)
```

Arguments

read.input list of arguments representing a methodology for acquiring the data of interest: the first argument is not named and will be passed to match.fun(); the other arguments will be passed to the result, and must include an argument named 'header'.

ext model file extension, e.g. 'mod' or 'ctl'
project project directory (can be expression)
nested whether model files are nested in eponymous directories
... passed to modelfile and link{datafile}

Value

logical

```
Other superset: generalize(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

initial.model 23

initial.model

Get Model Initial Estimates

Description

Gets model initial estimates.

Usage

```
## S3 method for class 'model'
initial(x, ...)
```

Arguments

```
x model ... dots
```

See Also

```
Other initial: initial(), initial<-(), initial<-.model()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% initial
```

initial<-.model</pre>

Set Upper Bounds for Model Initial Estimates

Description

Sets upper bounds for model initial estimates.

Usage

```
## S3 replacement method for class 'model'
initial(x) <- value</pre>
```

Arguments

```
x model value numeric
```

```
Other initial: initial(), initial.model(), initial<-()
```

24 likebut

likebut Modify a Model

Description

Makes a copy of a model in a corresponding directory. Problem statement is updated to reflect that the model is LIKE the reference model BUT different in some fundamental way.

Usage

```
likebut(
    x,
    but = "better",
    y = NULL,
    project = getOption("project", getwd()),
    nested = getOption("nested", TRUE),
    overwrite = FALSE,
    ext = getOption("modex", "ctl"),
    include = "\\.def$",
    update = FALSE,
    ...
)
```

Arguments

X	a model name, presumably interpretable as numeric
but	a short description of the characteristic difference from x
У	optional name for model to be created, auto-incremented by default
project	project directory (can be expression)
nested	model files nested in run-specific directories
overwrite	whether to overwrite y if it exists
ext	extension for the model file
include	regular expressions for files to copy to new directory
update	use final estimates of x as initial estimates of y
	passed arguments, including PsN runrecord elements (experimental)

Value

the value of y

```
runlog.character
```

lower.model 25

Examples

```
# Create a working project.
source <- system.file(package = 'nonmemica','project')
target <- tempdir()
target <- gsub('\\\','/',target) # for windows
source
target
file.copy(source,target,recursive = TRUE)
project <- file.path(target,'project','model')

# Point project option at working project
options(project = project)
library(magrittr)

# Derive models.
1001 %>% likebut('revised',y = 1002, overwrite=TRUE)

# At this point, edit 1002.ctl to match whatever 'revised' means.
# Then run it with NONMEM.
```

lower.model

Get Lower Bounds for Model Initial Estimates

Description

Gets lower bounds for model initial estimates.

Usage

```
## S3 method for class 'model'
lower(x, ...)
```

Arguments

```
x model ... dots
```

See Also

```
Other lower: lower(), lower<-(), lower<-.model()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% lower
```

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lower<-.model

Set Lower Bounds for Model Initial Estimates

Description

Sets lower bounds for model initial estimates.

Usage

```
## S3 replacement method for class 'model'
lower(x) <- value</pre>
```

Arguments

x model value numeric

See Also

```
Other lower: lower(), lower.model(), lower<-()
```

meta.character

Get Metadata for Character

Description

Gets metadata for character, treating it as a model name. Blends metadata from specifle with metadata from control stream, removing both exact duplicates as well as redefined values (with warning).

Usage

```
## S3 method for class 'character'
meta(x, simplify = TRUE, ...)
```

Arguments

x object

simplify logical: remove range information from guide text

... passed arguments

Value

data.frame

metaplot.character 27

See Also

```
Other superset: generalize(), ignored(), meta(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% meta
```

metaplot.character

Metaplot Character

Description

Plots character by treating as model name. A dataset is constructed by combining the meta version of the model input with a meta version of the model output and calling metaplot with the result.

Usage

```
## S3 method for class 'character'
metaplot(x, ..., groups, meta = match.fun("meta")(x), subset)
```

Arguments

```
    x object
    ... unquoted names of variables to plot, or other named arguments (passed)
    groups columns by which to group the dataset
    meta metadata; meta(x) by default
    subset a condition for filtering data
```

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

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Examples

```
library(magrittr)
library(metaplot)
options(project = system.file('project/model',package='nonmemica'))
## Not run:
1001 %>% metaplot(
   CWRESI, TAD, SEX,
   groups = c('ID','TIME'),
   subset = 'MDV == 0',
   yref = 0,
   ysmooth = TRUE
)
## End(Not run)
```

metaplot_character

Metaplot Character, Standard Evaluation

Description

Plots character by treating as model name. A dataset is constructed by combining the model input with a the model output and calling metaplot with the result.

Usage

```
metaplot_character(x, groups, meta = NULL, subset, var, ...)
```

Arguments

```
x object
groups columns by which to group the dataset
meta metadata; meta(x) by default
subset a condition for filtering data
var variables to plot
... passed arguments
```

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec.character(), superspec.numeric()
```

metasuperset 29

metasuperset

Retrieve Model Outputs with Metadata

Description

Retrieves model outputs with metadata.

Usage

```
metasuperset(
    x,
    groups,
    meta = match.fun("meta")(x, ...),
    subset = getOption("metasuperset_subset", NULL),
    ...
)
```

Arguments

```
x model name
groups vector of key column names in superset, e.g. USUBJID, TIME
meta metadata with column 'item' and possibly attributes such as 'label' and 'guide'
subset length-one character: a condition for filtering results, e.g. 'EVID == 0'
... passed arguments
```

Value

data.frame

See Also

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec.character(), superspec.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% metasuperset(c('ID','TIME')) %>% head
```

30 modelfile

modeldir

Identify the Directory for a Model

Description

Identifies the directory used by a model.

Usage

```
modeldir(x, ext, ...)
```

Arguments

```
x the model nameext model file extension... passed arguments
```

Value

character

See Also

```
Other path: datafile(), datafile.character(), datafile.numeric(), modelfile(), modelpath(), modelpath.character(), modelpath.numeric(), psn_options(), specfile(), specfile.character(), specfile.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% modeldir
```

modelfile

Identify the Modelfile for a Model

Description

Identifies the modelfile used by a model.

Usage

```
modelfile(x, ext = getOption("modex", "ctl"), ...)
```

modelpath 31

Arguments

```
x the model nameext model file extension... passed arguments
```

Value

character

See Also

```
Other path: datafile(), datafile.character(), datafile.numeric(), modeldir(), modelpath(), modelpath.character(), modelpath.numeric(), psn_options(), specfile(), specfile.character(), specfile.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% modelfile('xml')
```

modelpath

Resolve A Path to a Model-related File

Description

Resolves a path to a model-related file.

Usage

```
modelpath(x, ...)
```

Arguments

x object

... passed arguments

Value

character

```
Other path: datafile(), datafile.character(), datafile.numeric(), modeldir(), modelfile(), modelpath.character(), modelpath.numeric(), psn_options(), specfile(), specfile.character(), specfile.numeric()
```

32 modelpath.character

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% modelpath
```

modelpath.character

Resolve A Path to a Model-related File for Character

Description

Resolves a path to a model-related file, treating x as a model name. By default (ext is NULL) the run directory is returned. As of version 0.9.2, nested can be a function of ext and ... That returns logical.

Usage

```
## $3 method for class 'character'
modelpath(
    x,
    ext = NULL,
    project = getOption("project", getwd()),
    nested = getOption("nested", TRUE),
    ...
)
```

Arguments

```
x object
ext file extension, no leading dot
project project directory (can be expression)
nested whether model files are nested in eponymous directories
... passed arguments
```

Value

character

```
Other path: datafile(), datafile.character(), datafile.numeric(), modeldir(), modelfile(), modelpath(), modelpath.numeric(), psn_options(), specfile(), specfile.character(), specfile.numeric()
```

ninput 33

ninput

Calculate Number of Inputs

Description

Calculates number of inputs.

Usage

```
ninput(x, ...)
```

Arguments

x object

... passed arguments

See Also

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot.numeric(), metaplot.character(), metasuperset(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec.numeric()
```

ninput.character

Calculate Number of Inputs for Character

Description

Calculates number of inputs for character by treating as a model name.

Usage

```
## S3 method for class 'character'
ninput(x, ...)
```

Arguments

x character

... passed arguments

Value

integer

See Also

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot.character(), metasuperset(), ninput(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

ninput.numeric

Calculate Number of Inputs for Numeric

Description

Calculates number of inputs for numeric by coercing to character.

Usage

```
## S3 method for class 'numeric' ninput(x, ...)
```

Arguments

x numeric

... passed arguments

See Also

```
Other superset: generalize(), ignored(), meta(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput(), ninput(character(), shuffle(), superset(), superset(), superset(), supersec(), superspec(), superspe
```

```
nms_canonical.character
```

Generate Canonical Names for Character

Description

Generates canonical names for character by converting to parsed model.

Usage

```
## S3 method for class 'character' nms_{canonical}(x, ...)
```

nms_canonical.model 35

Arguments

```
x object of dispatch... passed arguments
```

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_canonical(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% nms_canonical
```

nms_canonical.model

Generate Canonical Names for Model

Description

Generates canonical names for a NONMEM control stream object. Canonical names indicate all and only the declared model parameters in lower-case conventional order (theta, omega row-major, sigma) with underscores and two-digit (or more) indices. E.g. theta_01, theta_02, omega_01_01, omega_02_01, omega_02_02, omega_01_01.

Usage

```
## S3 method for class 'model'
nms_canonical(x, ...)
```

Arguments

```
x a model designator
... passed arguments
```

Value

```
nms_canonical (character)
```

See Also

as.model

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric() nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

nms_canonical.nms_nonmem

Convert NONMEM Parameter Names to Canonical

Description

Converts nms_nonmem to nms_canonical.

Usage

```
## S3 method for class 'nms_nonmem'
nms_canonical(x, ...)
```

Arguments

x nms_nonmem

... ignored

Value

nms_canonical

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

nms_nonmem.character 37

nms_nonmem.character Generate NONMEM Names for Character

Description

Generates NONMEM names for numeric by converting to parsed model.

Usage

```
## S3 method for class 'character'
nms_nonmem(x, ...)
```

Arguments

x object of dispatch... passed arguments

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% nms_nonmem
```

nms_nonmem.model

Generate NONMEM Names for Model

Description

Generates NONMEM names for parameters declared in a NONMEM control stream object.

Usage

```
## S3 method for class 'model'
nms_nonmem(x, ...)
```

Arguments

```
x a model designator
... passed arguments
```

Value

```
nms_nonmem (character)
```

See Also

```
as.model
```

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% nms_nonmem
```

nms_nonmem.nms_canonical

Convert Canonical Parameter Names to NONMEM

Description

Converts nms_canonical to nms_nonmem.

Usage

```
## S3 method for class 'nms_canonical'
nms_nonmem(x, ...)
```

Arguments

```
x nms_canonical ignored
```

Value

nms_nonmem

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_pmx(), nms_pmx(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

Examples

```
# example code
```

nms_nonmem.nms_pmx

Convert pmxTools Names to NONMEM

Description

Converts nms_pmx to nms_nonmem. I.e., THETA1 stays THETA1, but OM1,1 becomes OMEGA(1,1).

Usage

```
## S3 method for class 'nms_pmx'
nms_nonmem(x, ...)
```

Arguments

```
x nms_pmx ignored
```

Value

```
nms_nonmem (character)
```

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_pmx.nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()

Other nm: nms_canonical.nms_pmx(), nms_pmx.nms_nonmem()
```

```
library(magrittr)
c(
    'THETA1',
    'OM1,1',
    'OM1,2',
    'SG1,1',
    'SG1,2'
) %>%
as_nms_pmx %>%
nms_canonical
```

nms_pmx.nms_canonical Convert Canonical Names to pmxTools

Description

Converts nms_canonical to nms_pmx. I.e., theta_01 becomes THETA1, and omega_01_01 becomes OM1,1.

Usage

```
## S3 method for class 'nms_canonical'
nms_pmx(x, ...)
```

Arguments

```
x nms_canonical ignored
```

Value

```
nms_pmx (character)
```

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_nonmem(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()
```

```
library(magrittr)
c(
   'theta_15',
   'omega_01_01',
   'omega_01_02',
   'sigma_01_01',
   'sigma_02_01'
) %>%
as_nms_canonical %>%
nms_pmx
```

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nms_pmx.nms_nonmem

Convert NONMEM Names to pmxTools

Description

Converts nms_nonmem to nms_pmx. I.e., THETA1 stays THETA1, but OMEGA(1,1) becomes OM1,1.

Usage

```
## S3 method for class 'nms_nonmem'
nms_pmx(x, ...)
```

Arguments

```
x nms_pmx
... ignored
```

Value

```
nms_nonmem (character)
```

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_psn(), nms_psn.character(), nms_psn.model(), nms_psn.numeric()

Other nm: nms_canonical.nms_pmx(), nms_nonmem.nms_pmx()
```

```
library(magrittr)
c(
    'THETA1',
    'OMEGA(1,1)',
    'OMEGA(1,2)',
    'SIGMA(1,1)',
    'SIGMA(1,2)'
) %>%
as_nms_pmx %>%
nms_canonical
```

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nms_psn.character

Generate PsN-style Names for Character

Description

Generates PsN-style names for numeric by converting to parsed model.

Usage

```
## S3 method for class 'character'
nms_psn(x, ...)
```

Arguments

```
x object of dispatch... passed arguments
```

See Also

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.model(), nms_psn.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% nms_psn
```

nms_psn.model

Generate PsN-style Names for Model

Description

Generates PsN-style names for parameters declared in a NONMEM control stream object. PsN uses NONMEM-style names, substituting a comment, if any: everything after the first semicolon, up to the second semicolon if present, without leading/trailing spaces/tabs.

Usage

```
## S3 method for class 'model'
nms_psn(x, ...)
```

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Arguments

x a model designator... passed arguments

Value

nms_psn (character)

See Also

as.model

```
Other nms: as_nms_canonical(), as_nms_nonmem(), as_nms_pmx(), as_nms_psn(), nms_canonical(), nms_canonical.character(), nms_canonical.model(), nms_canonical.nms_nonmem(), nms_canonical.nms_pmx(), nms_canonical.numeric(), nms_nonmem(), nms_nonmem.character(), nms_nonmem.model(), nms_nonmem.nms_canonical(), nms_nonmem.nms_pmx(), nms_nonmem.numeric(), nms_pmx(), nms_pmx.nms_canonical(), nms_pmx.nms_nonmem(), nms_psn(), nms_psn.character(), nms_psn.numeric()
```

nonmemica

Create and Evaluate NONMEM Models in a Project Context

Description

Nonmemica (emphasis like 'America') creates and evaluates NONMEM models in a project context.

Details

NONMEM (ICON Development Solutions) is software for nonlinear mixed effects modeling. The fundamental interface is a text file (control stream, typ. *.mod or *.ctl) that specifies model input, structure, and output. There are many add-on interfaces for NONMEM (see references for a few examples). However, much day-to-day modeling, even for R users, involves substantial manual interventions.

Nonmemica streamlines interactions with NONMEM. It adopts some established conventions and techniques (e.g. from PsN and metrumrg), but introduces others that may be useful. Principally, it parses existing control streams for systematic analysis and alteration. Relatively simple, single-problem control streams are supported; see the example.

Of course, NONMEM itself is licensed software that must be installed independently. Nonmemica is largely indifferent to how NONMEM is installed or invoked. However, several features depend on the *.xml output that NONMEM creates; make sure it is available. Also, the best-supported directory structure is that which has numbers for model names, with all model-specific files in eponymous subdirectories of a "project" directory. An example is given below.

Nonmemica adopts three control stream encoding conventions that merit special mention. First, the problem statement is encoded in the form //like/x//but/y// where x is a reference model name and y is a feature difference from the reference model (see likebut()). This allows any given model to be described by chaining together its legacy of features (use runlog(depenencies = TRUE, ...)), which

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generally works better than trying to describe it exhaustively in the model name. As of version 0.9.2, experimental support is available for natural-language problem statements of the form "like run1001 but fixed additive error".

Second, Nonmemica only needs a single output table (\$TABLE record). Be sure to use ONE-HEADER but avoid FIRSTONLY. Nonmemica will integrate model inputs and outputs, regardless of table counts, into one data.frame (see superset()).

Third, Nonmemica supports integrated metadata. With respect to model inputs, use package spec to store column metadata in a companion file (a data specification, e.g. *.spec). Keep the data file and data specification in a central location, not copied to the model directory. For model outputs (tabled items) supply column metadata directly in the control stream (or a *.def file; see example and help).

Nonmemica supports three global options: 'project' (default getwd()) is the parent directory of model-specific files or directories; 'nested' (default TRUE) tells whether model-specific files are nested within eponymous directories; 'modex' (default 'ctl') gives the file extension for control streams. In many cases you can pass these options to the relevant functions; but since they likely won't change for the scope of a given project, it saves effort to set them as global options (if they differ from the defaults) using e.g. options(project=).

Numbers make good names for models because it is never hard for you or the software to think of a new one. That said, model names are typically processed as character in Nonmemica. There are many generic functions with both numeric and character methods that simply assume the (length-one) argument you supply is a model name.

Author(s)

Maintainer: Tim Bergsma

 dergsmat@gmail.com>

References

NONMEM

Icon

PsN

Xpose

Wings for NONMEM

metrumrg

```
# Create a working project.
source <- system.file(package = 'nonmemica','project')
target <- tempdir()
target <- gsub('\\\\','/',target) # for windows
source
target
file.copy(source,target,recursive = TRUE)
project <- file.path(target,'project','model')
# Point project option at working project</pre>
```

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```
options(project = project)
# Load some packages
library(magrittr)
library(metaplot)
library(wrangle)
library(spec)
library(dplyr,warn.conflicts = FALSE)
# Identify features of a model.
1001 %>% modelpath
1001 %>% modeldir
1001 %>% modelfile
1001 %>% modelpath('xml')
1001 %>% datafile
datafile(1001) %matches% specfile(1001)
1001 %>% specfile
1001 %>% specfile %>% read.spec
1001 %>% as.model
1001 %>% as.model %>% comments
1001 %>% definitions
1001 %>% runlog(TRUE)
1001 %>% runlog
1001 %>% partab
1001 %>% num_parameters
1001 %>% nms_canonical
1001 %>% nms_psn
1001 %>% nms_nonmem
1001 %>% parameters
1001 %>% errors
1001 %>% as.model %>% initial
1001 %>% as.model %>% lower
1001 %>% as.model %>% upper
1001 %>% as.model %>% fixed
1001 %>% meta %>% class
1001 %>% meta
# Derive datasets.
1001 %>% superset %>% head
1001 %>% superset %>% filter(VISIBLE == 1) %>% group_by(ID,TIME) %>% status
1001 %>% metasuperset(c('ID','TIME')) %>% head
1001 %>% metasuperset(c('ID','TIME')) %>% sapply(attr,'label')
# Make diagnostic plots.
1001 %>% metaplot(
 CWRESI, TAD, SEX,
 groups = c('ID', 'TIME'),
 subset = 'MDV == 0',
 yref=0,
ysmooth = TRUE
1001 %>% metaplot(
 ETA1, SEX,
```

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```
ref = 0,
groups = c('ID', 'TIME'),
subset = 'MDV == 0'
1001 %>% metaplot(
SEX, ETA1,
ref = 0,
groups = c('ID','TIME'),
subset = 'MDV == 0'
1001 %>% metaplot(
ETA1, ETA2, ETA3,
groups = c('ID','TIME'),
subset = 'MDV == 0'
# Derive models.
1001 %>% likebut('revised',y = 1002, overwrite=TRUE )
# At this point, edit 1002.ctl to match whatever 'revised' means.
# Then run it with NONMEM and post-process results as above.
# Make ten new models with slightly different initial estimates.
1001 %>% tweak
```

offdiag.halfmatrix

Isolate Off-diagonal of Half Matrix

Description

Isolates off-diagonal of halfmatrix.

Usage

```
## S3 method for class 'halfmatrix' offdiag(x, ...)
```

Arguments

x object

... passed arguments

```
Other halfmatrix: as.data.frame.halfmatrix(), as.halfmatrix(), as.halfmatrix.default(), as.halfmatrix.halfmatrix(), as.matrix.halfmatrix(), half(), half.matrix(), is.square(), is.square.matrix(), offdiag(), ord(), ord.halfmatrix(), ord.matrix(), print.halfmatrix()
```

parameters.character 47

```
parameters.character Get Parameters for Character
```

Description

Gets parameters, treating character as model names. If x is length one, slightly more details are returned such as datafile, reference model, and feature. Otherwise results are bound together, one model per column. See estimates and errors for a more formal interface to model estimates and asymptotic standard errors.

Usage

```
## S3 method for class 'character'
parameters(x, simplify = FALSE, ...)
```

Arguments

```
x objectsimplify if x is length one and simplify is TRUE, return a named vectorpassed arguments
```

Value

data.frame

See Also

```
Other parameters: parameters(), parameters.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% parameters
```

partab

Create Parameter Table

Description

Creates a parameter table.

Creates a model parameter table from a partab object.

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Usage

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

Arguments

```
x partab ... ignored
```

Details

x can be numeric or character model name, assuming project is identified by argument or option. Just returns the object unmodified.

Methods (by class)

```
• partab(partab): partab method
```

See Also

```
partab.character
Other partab: partab.character(), partab.numeric()
Other partab: partab.character(), partab.numeric()
```

partab.character

Create a Parameter Table from Model Name

Description

Creates a parameter table from a model name. Pass the project argument or set the project option.

Usage

```
## S3 method for class 'character'
partab(
    x,
    verbose = FALSE,
    lo = "5",
    hi = "95",
    metafile = modelpath(x, "def", ...),
    xmlfile = modelpath(x, "xml", ...),
    ctlfile = modelfile(x, ...),
    bootcsv,
    strip.namespace = TRUE,
```

partab.character 49

```
skip = 28,
check.names = FALSE,
digits = 3,
ci = TRUE,
open = "(",
close = ")",
sep = ", ",
format = TRUE,
fields = getOption("fields", default = c("symbol", "label", "unit")),
relative = TRUE,
percent = relative,
nonzero = TRUE,
shrinkage = FALSE,
correlation = FALSE,
...
)
```

Arguments

x	a model name (numeric or character)
verbose	set FALSE to suppress messages
lo	the PsN bootstrap lower confidence limit (%)
hi	the PsN bootstrap upper confidence limit (%)
metafile	optional metadata for parameter table (see also: fields)
xmlfile	path to xml file
ctlfile	path to control stream
bootcsv	path to PsN bootstrap_results.csv
strip.namespace	
	whether to strip e.g. nm: from xml elements for easier xpath syntax
skip	number of lines to skip in bootstrap_results.csv
check.names	passed to bootstrap reader
digits	limits numerics to significant digits (use NULL to suppress)
ci	combine bootstrap lo and hi into an enclosed interval
open	first character for bootstrap interval
close	last character for bootstrap interval
sep	separator for bootstrap interval
format	format numerics as character
fields	metadata fields to read from control stream. See details.
relative	transform standard errors to relative standard errors: rse replaces se
percent	if relative is true, express as percent (else ignore): prse replaces se
nonzero	limit random effects to those with nonzero estimates
shrinkage	whether to include percent shrinkage on random effects
correlation	whether to include correlation of random effects (as percent if percent is true)
	passed to other functions

50 problem.character

Details

Normally you can just call the generic. Suitable defaults are supplied, but much customization is supported by means of arguments documented here and in called functions.

Metadata can be added to the parameter table two ways: as markup in the control stream, and as a *.def file in the model directory. See vignette('parameter-table') for details.

Value

object of class partab, data.frame

See Also

```
as.xml_document.character
as.bootstrap.character
as.model.character
as.csv
Other partab: partab(), partab.numeric()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% partab
1001 %>% partab(shrinkage = TRUE, correlation = TRUE)
```

problem.character

Identify the Model Problem Statement for Character

Description

Identifies the model problem statement for character (model name).

Usage

```
## S3 method for class 'character'
problem(x, ...)
```

Arguments

```
x object... passed arguments
```

Value

character

psn_nested 51

See Also

```
Other problem: as.problem(), problem(), problem.numeric(), problem_()
```

psn_nested

PsN Model File is Nested

Description

Check whether a particular file extension corresponds to a file that is nested within a subdirectory using default PsN conventions.

Usage

```
psn_nested(x, ...)
```

Arguments

```
x character, a file extension, without dot.... ignored
```

Value

logical

Examples

```
psn_nested('mod')
```

psn_options

Set PsN Options

Description

Sets PsN-style directory and control stream options. Supports control streams with semicolon-delimited metadata including symbol, unit, transform, and label. Expects model files to be found in nested directory, except for *.mod and *.lst.

Usage

```
psn_options(
  project = "NONMEM",
  modex = "mod",
  fields = c("symbol", "unit", "transform", "label"),
  nested = psn_nested,
  ...
)
```

52 relativizePath

Arguments

project character, path to project directory

modex character, extension for model control stream (no dot)

fields character

nested logical, or function of file extension returning logical

... ignored

Value

```
used for side-effects (sets options 'fields' and 'nested')
```

See Also

```
Other path: datafile(), datafile.character(), datafile.numeric(), modeldir(), modelfile(), modelpath(), modelpath.character(), modelpath.numeric(), specfile(), specfile.character(), specfile.numeric()
```

Examples

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

relativizePath

Relativize a Path

Description

Relativizes a path.

Usage

```
relativizePath(x, dir = getwd(), sep = "/", ...)
```

Arguments

```
x a file pathdir a reference directorysep path separator
```

... ignored arguments

Details

x and dir are first normalized, then x is expressed relative to dir. If x and dir are on different drives (i.e. C:/D:/) x is returned as an absolute path.

resolve 53

resolve

Resolve File Path

Description

Resolves a file path. Returns the path if absolute. If relative, concatenates the directory and file.

Usage

```
resolve(file, dir)
```

Arguments

file path to a file

dir reference directory for a relative file path

Value

character

rosetta

Translate Parameter Names

Description

Translate among various idioms for expressing parameter names

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))

# we generate some nonmem parameter names in nonmem format
1001 %>% nms_nonmem -> nonmem
nonmem

# from these we generate canonical and pmxTools equivalents
canonical <- nms_canonical(nonmem)
pmxtools <- nms_pmx(nonmem)
canonical
pmxtools

# We demonstrate equivalence
stopifnot(identical(nonmem, nms_nonmem(canonical)))
stopifnot(identical(nonmem, nms_nonmem(pmxtools)))
stopifnot(identical(canonical, nms_canonical(nonmem)))
stopifnot(identical(canonical, nms_canonical(pmxtools)))</pre>
```

54 runlog.character

```
stopifnot(identical(pmxtools, nms_pmx(nonmem)))
stopifnot(identical(pmxtools, nms_pmx(canonical)))

# on-the-fly conversions
nonmem %>% class
nonmem %>% nms_pmx
nonmem %>% nms_canonical
nonmem %>% nms_canonical
nonmem %>% nms_canonical %>% nms_pmx
nonmem %>% nms_canonical %>% nms_pmx
nonmem %>% nms_canonical %>% nms_pmx %>% nms_nonmem

# comparison
data.frame(
can = I(canonical),
non = I(nonmem),
pmx = I(pmxtools),
psn = I(nms_psn(1001))
)
```

runlog.character

Create a Runlog for Character

Description

Creates a Runlog for character by treating x as modelname(s).

Usage

```
## S3 method for class 'character'
runlog(x, dependencies = FALSE, digits = 3, places = 0, ...)
```

Arguments

```
    x object
    dependencies whether to log runs in lineage(s) as well
    digits significance for parameters
    places rounding for objective function
    passed arguments
```

Value

data.frame

```
likebut
```

```
Other runlog: runlog(), runlog.numeric()
```

safe_join 55

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
# likebut(2001,'2 cmt', 2002)  # edit manually, then ...
# likebut(2002,'add. err.', 2003)  # edit manually, then ...
# likebut(2003,'allo. WT on CL',2004)  # edit manually, then ...
# likebut(2004,'estimate allometry', 2005)  # edit manually, then ...
# likebut(2005,'SEX on CL', 2006)  # edit manually, then ...
# likebut(2006,'full block omega', 2007)  # edit manually, then run all
2007 %>% runlog(dependencies = TRUE)
```

safe_join

Join Data Safely

Description

Joins data safely. Generic, with method for data.frame.

Usage

```
safe_join(x, ...)
```

Arguments

```
x object of dispatch... arguments to methods
```

See Also

```
safe_join.data.frame
Other safe_join: safe_join.data.frame()
```

```
safe_join.data.frame Join Data Frames Safely
```

Description

Joins data frames safely. I.e., a left join that cannot alter row order or number. Supports the case where you only intend to augment existing rows with additional columns and are expecting singular matches. Gives an error if row order or number would have been altered by a left join.

Usage

```
## S3 method for class 'data.frame'
safe_join(x, y, ...)
```

56 shuffle

Arguments

```
x data.frame
y data.frame
```

... passed to dplyr::left_join

See Also

```
Other safe_join: safe_join()
```

Examples

```
library(magrittr)
x <- data.frame(code = c('a','b','c'), value = c(1:3))
y <- data.frame(code = c('a','b','c'), roman = c('I','II','III'))
x %>% safe_join(y)
try(
x %>% safe_join(rbind(y,y))
)
```

shuffle

Move the Columns of a Data Frame Relative to Each Other

Description

Move the columns of a data frame relative to each other.

Usage

```
shuffle(x, who, after = NA, ...)
```

Arguments

x data.frame

who a character vector of column names to move, or a logical vector of length names(x),

or a vector of indices

after column after which to put who: may be character, integer, NA, or NULL

... ignored

Value

data.frame

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), superset(), superset.character(), superset.numeric(), superspec(), superspec.character(), superspec.numeric()
```

specfile.character 57

specfile.character

Identify the Data Specification File for a Model

Description

Identifies the data specification file associated with the datafile used by a model. Locates the datafile specified in the control stream, and substitutes a different extension.

Usage

```
## S3 method for class 'character'
specfile(x, find = "\\.csv$", use = ".spec", ...)
```

Arguments

x the model name

find file extension to replace

use file extension to use

... pass ext over-ride default file extension in datafile()

Value

character

See Also

datafile

```
Other path: datafile(), datafile.character(), datafile.numeric(), modeldir(), modelfile(), modelpath(), modelpath.character(), modelpath.numeric(), psn_options(), specfile(), specfile.numeric()
```

```
library(spec)
source <- system.file(package = 'nonmemica','project')
target <- tempdir()
target <- gsub('\\\','/',target) # for windows
file.copy(source,target,recursive = TRUE)
project <- file.path(target,'project','model')
options(project = project)
library(magrittr)
1001 %>% datafile
datafile(1001) %matches% specfile(1001)
1001 %>% specfile
1001 %>% specfile %>% read.spec
```

58 superset.character

superset.character Coerce to Superset from Character

Description

Coerces to superset from character, treating x as a model name.

Usage

```
## S3 method for class 'character'
superset(
    x,
    read.input = list(read.csv, header = TRUE, as.is = TRUE),
    read.output = list(read.table, header = TRUE, as.is = TRUE, skip = 1, comment.char =
        "", check.names = FALSE, na.strings = c("", "\\s", ".", "NA")),
    include = character(0),
    exclude = character(0),
    rename = NULL,
    digits = 5,
    visible = "VISIBLE",
    after = NULL,
    groups = character(0),
    imputation = generalize,
    ...
)
```

Arguments

x	object
read.input	a methodology for acquiring the input
read.output	a methodology for acquiring the output
include	column names in output to consider adding
exclude	column names in output to reject
rename	logical: whether to keep and rename columns with re-used names
digits	significant digits for assessing informativeness when exclusive=NULL
visible	a name for the flag column indicating visibility
after	place new columns after this column; at end by default (NULL); TRUE places them after last model-visible column (see input statement)
groups	character vector of groupings within which any imputations will be performed
imputation	a list of functions (or arguments to match.fun()) to perform imputations within cells defined by groups: e.g. generalize, forbak, etc (to be tried in succession for new columns only).
	passed arguments

superset.character 59

Details

Given a model name, (project passed or set as global option) superset() figures out the run directory and location of a NONMEM control stream. It reads the control stream to identify the run-time location of input and output files, as well as the "ignore" (and/or "accept") criteria that relate extent of input records to extent of output records. 'read.input' and 'read.output' are lists consisting of functions and arguments appropriate for reading input and output file formats, respectively. The ignore criteria will be reconstructed per row so that output can be mapped unambiguously to input. A column named VISIBLE is bound to the input data, showing 1 where a record was visible to NONMEM, and 0 otherwise. During integration, naming convention of the input is retained, and output column names are mapped by position, using the control stream input criteria. Output tables are restored to input dimensions using the "ignore" criteria, then checked for length: currently, superset ignores output tables having fewer rows than the input, as well as output tables whose row count is not a multiple of input row count. Output tables may contain versions of input columns. Disposition depends on the values of include, exclude, and rename. If include has length, other columns are excluded. Then, if exclude has length, these columns are excluded. Then, if rename is FALSE all remaining columns with re-used names will be dropped. If TRUE, such columns will be renamed (*.n, where n is table number). If NULL, only informative columns will be retained and renamed. A column is informative if any element is informative. An element is informative if it is newly generated (not NA and not zero, but original is NA) or if it is an alteration (non-NA, and different from non-NA original). If the column pair can be interpreted as numeric, "different" is determined using only the first digits digits. Only the first instance of any column among successive output tables is retained. In the control stream, avoid use of FIRSTONLY, as this alters the number of rows.

Value

superset: a data.frame where row count is a multiple of (typically equal to) input row count.

See Also

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.numeric(), superspec.character(), superspec.numeric()
```

```
library(magrittr)
library(dplyr)
library(wrangle)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% superset %>% head
1001 %>% superset %>% filter(VISIBLE == 1) %>% group_by(ID,TIME) %>% status
1001 %>% ignored %>% table
```

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superspec

Create Specification for Model Inputs and Outputs

Description

Create a specification for the result of superset().

Usage

```
superspec(x, ...)
```

Arguments

```
x object... passed arguments
```

See Also

```
superspec.character
```

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec.character(), superspec.numeric()
```

superspec.character

Create Specification for Model Inputs and Outputs From Character

Description

Create a specification for the result of superset() from character by treating as a model name. By default, gives a spec template for superset(x). Tries to supplement with labels and units from parent specification, if it exists. Tries to supplement with any additional labels and units in definitions(x). Defers to actual data if provided. Specify exclusive, visible, and after as for superset.

Usage

```
## S3 method for class 'character'
superspec(
    x,
    include = character(0),
    exclude = character(0),
    rename = NULL,
    visible = "VISIBLE",
    after = NULL,
    data = NULL,
    ...
)
```

superspec.numeric 61

Arguments

X	character
include	column names in output to consider adding
exclude	column names in output to reject
rename	logical: whether to keep and rename columns with re-used names
visible	a name for the flag column indicating visibility
after	place new columns after this column; at end by default (NULL); TRUE places them after
data	an alternative dataset on which to model the specification
	passed arguments

See Also

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), superspec(), superspec.numeric()
```

superspec.numeric

Create Specification for Model Inputs and Outputs From Numeric

Description

Create a specification for the result of superset() from numeric by coercing to character.

Usage

```
## S3 method for class 'numeric'
superspec(x, ...)
```

Arguments

x numeric ... passed arguments

```
Other superset: generalize(), ignored(), meta(), meta.character(), meta.numeric(), metaplot.character(), metaplot.numeric(), metaplot_character(), metasuperset(), ninput(), ninput.character(), ninput.numeric(), shuffle(), superset(), superset.character(), superset.numeric(), supersec(), superspec(), superspec.character()
```

62 tad

tad

Calculate Time Since Most Recent Dose

Description

Calculate time since most recent dose. Considers ADDL, but may not work with simultaneous dose records.

Usage

```
tad(
    x,
    dose = rep(FALSE, length(x)),
    addl = rep(0, length(x)),
    ii = rep(0, length(x)),
    index = rep(1, length(x)),
    pre = TRUE,
    ...
)
```

Arguments

```
x a numeric vector of event times

dose length x logical indicating which of x are dose times

addl length x integer: number of additional doses

ii length x numeric: interdose interval for addl

index length x factor (optional) indicating subgroups to evaluate

pre assume that simultaneous sample precedes implied dose

... passed to tod()
```

Value

numeric

See Also

```
tod
Other tad: tod()
```

```
data(tad1)
x <- tad1
head(x)
x$tad <- tad(
    x = x$TIME,</pre>
```

tad1 63

```
dose = x$EVID %in% c(1,4) & is.na(x$C),
  addl = x$ADDL,
  ii = x$II,
  index = x$ID
)
head(x)
```

tad1

A NONMEM-like Dataset

Description

A dataset showing dose and and observation records for several subjects. Doses are duplicated across compartments 1 and 2 as for mixed absorption modeling.

Usage

```
data(tad1)
```

Details

- C. An exclusion flag, NA by default, or 'C'.
- ID. Integer subject identifier.
- TIME. Numeric event time (h).
- EVID. Event type identifier: observation (0) or dose (1).
- CMT. Event compartment: dose (1), central (2) or peripheral (4).
- AMT. Amount of dose (mg).
- RATE. NONMEM RATE item.
- ADDL. Number of additional doses, or NA for observations.
- II. Interdose interval for additional doses, or NA for observations.
- DV. Observation placeholder.

tod

Calculate Time of Most Recent Dose

Description

Calculates time of most recent dose.

Usage

```
tod(x, ref, addl, ii, pre = T, ...)
```

64 tweak.default

Arguments

X	a numeric vector of event times
ref	length x vector of reference dose times
addl	length x integer: number of additional doses
ii	length x numeric: interdose interval for addl
pre	assume that simultaneous sample precedes implied dose
	ignored

Value

numeric

See Also

tad

Other tad: tad()

tweak.default

Tweak a Model by Default

Description

Tweaks a model by jittering initial estimates. Creates a new model directory in project context and places the model there. Copies helper files as well. Expects that x is a number. Assumes nested directory structure (run-specific directories).

Usage

```
## Default S3 method:
tweak(
    x,
    project = getOption("project", getwd()),
    ext = getOption("modex", "ctl"),
    start = NULL,
    n = 10,
    include = ".def$",
    ...
)
```

tweak.model 65

Arguments

object

project project directory (can be expression)
ext file extension for control streams

start a number to use as the first modelname

n the number of variants to generate (named start:n) include regular expressions for files to copy to new directory pass ext to over-ride default model file extension

Value

character: vector of names for models created

See Also

```
Other tweak: tweak(), tweak.init(), tweak.inits(), tweak.model()
```

tweak.model

Tweak Model

Description

Tweaks model.

Usage

```
## S3 method for class 'model'
tweak(x, sd = 0.13, digits = 3, ...)
```

Arguments

```
x model sd numeric digits integer
```

... passed arguments

Value

model

```
Other tweak: tweak(), tweak.default(), tweak.init(), tweak.inits()
```

66 updated.character

Examples

```
# Create a working project.
source <- system.file(package = 'nonmemica','project')
target <- tempdir()
target <- gsub('\\\','/',target) # for windows
source
target
file.copy(source,target,recursive = TRUE)
project <- file.path(target,'project','model')

# Point project option at working project
options(project = project)
library(magrittr)

# Make ten new models with slightly different initial estimates.
1001 %>% tweak
```

updated.character

Create the Updated Version of Character

Description

Creates the updated version of character by treating as a modelname. Parses the associated control stream and ammends the initial estimates to reflect model results (as per xml file).

Usage

```
## S3 method for class 'character' updated(x, initial = estimates(x, ...), parse = TRUE, verbose = FALSE, ...)
```

Arguments

```
x character
initial values to use for initial estimates (numeric)
parse whether to parse the initial estimates, etc.
verbose extended messaging
... passed arguements
```

Value

model

See Also

Other updated: updated(), updated.numeric()

upper.model 67

upper.model

Get Upper Bounds for Model Initial Estimates

Description

Gets upper bounds for model initial estimates.

Usage

```
## S3 method for class 'model'
upper(x, ...)
```

Arguments

```
x model ... dots
```

See Also

```
Other upper: upper(), upper<-(), upper<-.model()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% as.model %>% upper
```

upper<-.model

Set Upper Bounds for Model Initial Estimates

Description

Sets upper bounds for model initial estimates.

Usage

```
## S3 replacement method for class 'model'
upper(x) <- value</pre>
```

Arguments

```
x model value numeric
```

```
Other upper: upper(), upper.model(), upper<-()
```

68 xpath.default

xpath

Evaluate Xpath Expression

Description

Evaluates an xpath expression.

Usage

```
xpath(x, ...)
```

Arguments

x xml_document
... passed arguments

Details

The resulting nodeset is scavenged for text, and coerced to best of numeric or character.

See Also

```
Other xpath: as.xml_document(), as.xml_document.character(), as.xml_document.numeric(), xpath.default(), xpath.xml_document()
```

Examples

```
library(magrittr)
options(project = system.file('project/model',package='nonmemica'))
1001 %>% xpath('//etashrink/row/col')
```

xpath.default

Evaluate xpath Expression in Default Context

Description

Coerces x to xml_document and evaluates.

Usage

```
## Default S3 method:
xpath(x, ...)
```

Arguments

```
x default
```

... passed arguments

xpath.xml_document 69

Value

vector

See Also

```
Other xpath: as.xml_document(), as.xml_document.character(), as.xml_document.numeric(), xpath(), xpath.xml_document()
```

xpath.xml_document

Evaluate xpath Expression in Document Context

Description

Evaluates an xpath expression for a given document.

Usage

```
## S3 method for class 'xml_document'
xpath(x, xpath, ...)
```

Arguments

```
x xml_document
xpath xpath expression to evaluate
```

... ignored

Details

The resulting nodeset is scavenged for text, and coerced to best of numeric or character.

Value

vector

```
Other xpath: as.xml_document(), as.xml_document.character(), as.xml_document.numeric(), xpath(), xpath.default()
```

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