

Package ‘NMdata’

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Type Package

Title Preparation, Checking and Post-Processing Data for PK/PD Modeling

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Description Efficient tools for preparation, checking and post-processing of data in PK/PD (pharmacokinetics/pharmacodynamics) modeling, with focus on use of Nonmem. Helps with trivial but tedious tasks and tries to identify errors to save time on debugging. Implemented in 'data.table', but easily integrated with 'base' and 'tidyverse'.

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cc

Create character vectors without quotation marks

Description

When creating character vectors with several elements, it becomes a lot of quotes to type. `cc` provides a simple way to skip the quotes - but only for simple strings.

Usage

```
cc(...)
```

Arguments

... The unquoted names that will become character values in the returned vector.

Details

Don't use cc with any special characters - only alphanumerics and no spaces supported.

Examples

```
cc(a,b,`a b`)
cc(a,b,"a b")
## be careful with spaces and special characters
cc( d)
cc(" d")
cc()
```

compareCols

Compare elements in lists with aim of combining

Description

Useful interactive tool when merging or binding objects together. It lists the names of elements that differ in presence or class across multiple datasets. Before running rbind, you may want to check the compatibility of the data.

Usage

```
compareCols(
  ...,
  keepNames = TRUE,
  testEqual = FALSE,
  diff.only = TRUE,
  cols.wanted,
  fun.class = base::class,
  quiet,
  as.fun
)
```

Arguments

... objects which element names to compare

keepNames If TRUE, the original dataset names are used in reported table. If not, generic x1, x2,... are used. The latter may be preferred for readability.

testEqual Do you just want a TRUE/FALSE to whether the names of the two objects are the same? Default is FALSE which means to return an overview for interactive use. You might want to use TRUE in programming. However, notice that this check may be overly rigorous. Many classes are compitable enough (say numeric and integer), and compareCols doesn't take this into account.

<code>diff.only</code>	If TRUE, don't report columns where no difference found. Default is TRUE if number of data sets supplied is greater than one. If only one data set is supplied, the full list of columns is shown by default.
<code>cols.wanted</code>	Columns of special interest. These will always be included in overview and indicated by a prepended * to the column names. This argument is often useful when you start by defining a set of columns that you want to end up with by combining a number of data sets.
<code>fun.class</code>	the function that will be run on each column to check for differences. <code>base::class</code> is default. Notice that the alternative <code>base::typeof</code> is different in certain ways. For instance, <code>typeof</code> will not report a difference on numeric vs <code>difftime</code> . You could basically submit any function that takes a vector and returns a single value.
<code>quiet</code>	The default is to give some information along the way on what data is found. But consider setting this to TRUE for non-interactive use. Default can be configured using <code>NMdataConf</code> .
<code>as.fun</code>	A function that will be run un the result before returning. If first input data set is a <code>data.table</code> , the default is to return a <code>data.table</code> , if not the default is to return a <code>data.frame</code> . Use whatever to get what fits in with your workflow. Default can be configured with <code>NMdataConf</code> .

Details

tecnically, this function compares classes of elements in lists. However, in relation to `NMdata`, this will most of the time be columns in `data.frames`.

Value

A `data.frame` with an overview of elementes and their classes of objects in ... Class as defined by `as.fun`.

See Also

Other DataWrangling: [dims\(\)](#), [listMissings\(\)](#)

`dims`

Get dimensions of multiple objects

Description

Get dimensions of multiple objects

Usage

```
dims(..., list.data, keepNames = TRUE, as.fun = NULL)
```

Arguments

<code>...</code>	data sets
<code>list.data</code>	As alternative to <code>...</code> , you can supply the data sets in a list here.
<code>keepNames</code>	If TRUE, the original dataset names are used in reported table. If not, generic <code>x1, x2,...</code> are used. The latter may be preferred for readability in some cases.
<code>as.fun</code>	A function that will be run un the result before returning. If first input data set is a <code>data.table</code> , the default is to return a <code>data.table</code> , if not the default is to return a <code>data.frame</code> . Use whatever to get what fits in with your workflow. Default can be configured with <code>NMdataConf</code> .

Value

A `data.frame` with dimensions of objects in `...` Actual class defined by `as.fun`.

See Also

Other DataWrangling: [compareCols\(\)](#), [listMissings\(\)](#)

egdt	<i>Expand grid of data.tables</i>
------	-----------------------------------

Description

Expand grid of `data.tables`

Usage

```
egdt(dt1, dt2, quiet)
```

Arguments

<code>dt1</code>	a <code>data.table</code> .
<code>dt2</code>	another <code>data.table</code> .
<code>quiet</code>	The default is to give some information along the way on what data is found. But consider setting this to TRUE for non-interactive use. Default can be configured using <code>NMdataConf</code> .

Details

Merging works mostly similarly for `data.table` and `data.frame`. However, for `data.frame` the merge must be done by one or more columns. This means that the convenient way to expand all combinations of all rows in two `data.frames` is not available for `data.tables`. This functions provides that functionality. It always returns `data.tables`.

Value

a `data.table` that expands combinations of rows in `dt1` and `dt2`.

Examples

```
df1 <- data.frame(a=1:2,b=3:4)
df2 <- data.frame(c=5:6,d=7:8)
merge(df1,df2)
library(data.table)
## This is not possible
## Not run:
merge(as.data.table(df1),as.data.table(df2),allow.cartesian=TRUE)

## End(Not run)
## Use egdt instead
egdt(as.data.table(df1),as.data.table(df2))
```

findCovs

Extract columns that vary within values of other columns

Description

This function provides an automated method to extract covariate-like columns. The user decides which columns these variables cannot vary within. So if you have repeated measures for each ID, this function can find the columns that are constant within ID and their unique values for each ID. Or, you can provide a combination of id.cols, say ID and STUDY, and get variables that do not vary within unique combinations of these.

Usage

```
findCovs(data, by = NULL, cols.id, as.fun = NULL)
```

Arguments

data	data.frame in which to look for covariates
by	covariates will be searched for in combinations of values in these columns. Often by will be either empty or ID. But it can also be both say c("ID","DRUG") or c("ID","TRT").
cols.id	Deprecated. Use by instead.
as.fun	The default is to return a data.table if data is a data.table and return a data.frame in all other cases. Pass a function in as.fun to convert to something else. If data is not a data.table, the default can be configured using NMdataConf.

Value

a data set with one observation per combination of values of variables listed in by.

See Also

Other DataCreate: [NMorderColumns\(\)](#), [NMstamp\(\)](#), [findVars\(\)](#), [flagsAssign\(\)](#), [flagsCount\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

Examples

```

dt1=data.frame(ID=c(1,1,2,2),
               OCC=c(1,2,1,2),
               ## ID level
               eta1=c(1,1,3,3),
               ## occasion level
               eta2=c(1,3,1,5),
               ## not used
               eta3=0
               )
## model level
findCovs(dt1)
## ID level
findCovs(dt1,"ID")
## actual ID level
findVars(findCovs(dt1,"ID"))
## occasion level
findCovs(findVars(dt1,"ID"),c("ID","OCC"))
## Based on a "real data example"
dat <- NMscanData(system.file("examples/nonmem/xgxr001.lst", package = "NMdata"))
findCovs(dat,by="ID")
### Without an ID column we get non-varying columns
findCovs(dat)

```

findVars	<i>Extract columns that vary within values of other columns in a data.frame</i>
----------	---

Description

If you want to look at the variability of a number of columns and you want to disregard those that are constant. Like for findCovs, by can be of arbitrary length.

Usage

```
findVars(data, by = NULL, cols.id, as.fun = NULL)
```

Arguments

data	data.frame in which to look for covariates
by	optional covariates will be searched for in combinations of values in these columns. Often by will be either empty or ID. But it can also be both say c("ID","DRUG") or c("ID","TRT").
cols.id	Deprecated. Use by instead.
as.fun	The default is to return a data.table if data is a data.table and return a data.frame in all other cases. Pass a function in as.fun to convert to something else. If data is not a data.table, the default can be configured using NMdataConf.

Details

Use this to exclude columns that are constant within by. If by=ID, this could be to get only time-varying covariates.

Value

a data set with as many rows as in data.

See Also

Other DataCreate: [NMorderColumns\(\)](#), [NMstamp\(\)](#), [findCovs\(\)](#), [flagsAssign\(\)](#), [flagsCount\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

Examples

```
dt1 <- data.frame(ID=c(1,1,2,2),
                  OCC=c(1,2,1,2),
                  ## ID level
                  eta1=c(1,1,3,3),
                  ## occasion level
                  eta2=c(1,3,1,5),
                  ## not used
                  eta3=0
                  )
## model level
findCovs(dt1)
## ID level
findCovs(dt1,"ID")
## actual ID level
findVars(findCovs(dt1,"ID"))
## occasion level
findCovs(findVars(dt1,"ID"),c("ID","OCC"))
```

flagsAssign

Assign exclusion flags to a dataset based on specified table

Description

The aim with this function is to take a (say PK) dataset and a pre-specified table of flags, assign the flags automatically.

Usage

```
flagsAssign(
  data,
  tab.flags,
  subset.data,
  col.flagn,
```



```

    col.flagc,
    flags.increasing = FALSE,
    grp.incomp = "EVID",
    flagc.0 = "Analysis set",
    as.fun = NULL
)

```

Arguments

<code>data</code>	The dataset to assign flags to.
<code>tab.flags</code>	A data.frame containing at least these named columns: FLAG, flag, condition. Condition is disregarded for FLAG==0. FLAG must be numeric and non-negative, flag and condition are characters.
<code>subset.data</code>	An optional string that provides a subset of data to assign flags to. A common example is <code>subset="EVID==0"</code> to only assign to observations. Numerical and character flags will be missing in rows that are not matched by this subset.
<code>col.flagn</code>	The name of the column containing the numerical flag values in <code>tab.flags</code> . This will be added to <code>data</code> . Default value is FLAG and can be configured using <code>NMdataConf</code> .
<code>col.flagc</code>	The name of the column containing the character flag values in <code>tab.flags</code> . This will be added to <code>data</code> . Default value is flag and can be configured using <code>NMdataConf</code> .
<code>flags.increasing</code>	The flags are applied by either decreasing (default) or increasing value of <code>col.flagn</code> . Decreasing order means that conditions associated with higher values of <code>col.flagn</code> will be evaluated first. By using decreasing order, you can easily adjust the Nonmem IGNORE statement from <code>IGNORE(FLAG.NE.0)</code> to say <code>IGNORE(FLAG.GT.10)</code> if BLQ's have FLAG=10, and you decide to include these in the analysis.
<code>grp.incomp</code>	Column(s) that distinct incompatible subsets of data. Default is "EVID" meaning that if different values of EVID are found in <code>data</code> , the function will return an error. This is a safeguard not to mix data unintentionally when counting flags.
<code>flagc.0</code>	The character flag to assign to rows that are not matched by exclusion conditions (numerical flag 0).
<code>as.fun</code>	The default is to return <code>data.tables</code> if input data is a <code>data.table</code> , and return a <code>data.frame</code> for all other input classes. Pass a function in <code>as.fun</code> to convert to something else. If <code>return.all=FALSE</code> , this is applied to <code>data</code> and <code>tab.flags</code> independently.

Details

`dt.flags` must contain a column with numerical exclusion flags, one with character exclusion flags, and one with a expressions to evaluate for whether to apply the exclusion flag. The flags are applied sequentially, by increasing value of the numerical exclusion flag.

Value

The dataset with flags added. Class as defined by `as.fun`. See parameter `flags.return` as well.

See Also

Other DataCreate: [NMorderColumns\(\)](#), [NMstamp\(\)](#), [findCovs\(\)](#), [findVars\(\)](#), [flagsCount\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

Examples

```
pk <- readRDS(file=system.file("examples/data/xgxr2.rds",package="NMdata"))
dt.flags <- data.frame(
  flagn=10,
  flagc="Below LLOQ",
  condition=c("BLQ==1")
)
pk <- flagsAssign(pk,dt.flags,subset.data="EVID==0",col.flagn="flagn",col.flagc="flagc")
pk <- flagsAssign(pk,subset.data="EVID==1",flagc.0="Dosing",
  col.flagn="flagn",col.flagc="flagc")
unique(pk[,c("EVID","flagn","flagc","BLQ")])
flagsCount(pk[EVID==0],dt.flags,col.flagn="flagn",col.flagc="flagc")
```

flagsCount

Create an overview of number of retained and discarded datapoints.

Description

Generate an overview of number of observations disregarded due to different reasons. And how many are left after each exclusion flag.

Usage

```
flagsCount(
  data,
  tab.flags,
  file,
  col.id = "ID",
  col.flagn,
  col.flagc,
  by = NULL,
  flags.increasing = FALSE,
  flagc.0 = "Analysis set",
  name.all.data = "All available data",
  grp.incomp = "EVID",
  save = TRUE,
  as.fun = NULL
)
```

Arguments

<code>data</code>	The dataset including both FLAG and flag columns.
<code>tab.flags</code>	A data.frame containing at least these named columns: FLAG, flag, condition. Condition is disregarded for FLAG==0.
<code>file</code>	A file to write the table of flag counts to. Will probably be removed and put in a separate function.
<code>col.id</code>	The name of the subject ID column. Default is "ID".
<code>col.flagn</code>	The name of the column containing the numerical flag values in tab.flags. This will be added to data. Use the same as when flagsAssign was called (if that was used). Default value is FLAG and can be configured using NMdataConf.
<code>col.flagc</code>	The name of the column containing the character flag values in data and tab.flags. Use the same as when flagsAssign was called (if that was used). Default value is flag and can be configured using NMdataConf.
<code>by</code>	An optional column to group the counting by. This could be "STUDY", "DRUG", "EVID", or a combination of multiple columns.
<code>flags.increasing</code>	The flags are applied by either decreasing (default) or increasing value of col.flagn. By using decreasing order, you can easily adjust the Nonmem IGNORE statement from IGNORE(FLAG.NE.0) to say IGNORE(FLAG.GT.10) if BLQ's have FLAG=10, and you decide to include these in the analysis.
<code>flagc.0</code>	The character flag to assign to rows that are not matched by exclusion conditions (numerical flag 0).
<code>name.all.data</code>	What to call the total set of data before applying exclusion flags. Default is "All available data".
<code>grp.incomp</code>	Column(s) that distinct incompatible subsets of data. Default is "EVID" meaning that if different values of EVID are found in data, the function will return an error. This is a safeguard not to mix data unintentionally when counting flags.
<code>save</code>	Save file? Default is TRUE, meaning that a file will be written if file argument is supplied.
<code>as.fun</code>	The default is to return a data.table if input data is a data.table, and return a data.frame for all other input classes. Pass a function in as.fun to convert to something else. If data is not a data.table, default can be configured using NMdataConf.

Details

This function is used to count flags as assigned by the flagsAssign function.

Notice that the character flags reported in the output table are taken from tab.flags. The data column named by the value of col.flagc (default is flag) is not used.

In the returned table, N.discarded is the difference in number of subjects since previous step. If two is reported, it can mean that the remaining one observation of these two subjects are discarded due to this flag. The majority of the samples can have been discarded by earlier flags.

Value

A summary table with number of discarded and retained subjects and observations when applying each condition in the flag table. "discarded" means that the reduction of number of observations and subjects resulting from the flag, "retained" means the numbers that are left after application of the flag. The default is "both" which will report both. Class as defined by as.fun.

See Also

Other DataCreate: [NMorderColumns\(\)](#), [NMstamp\(\)](#), [findCovs\(\)](#), [findVars\(\)](#), [flagsAssign\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

Examples

```
pk <- readRDS(file=system.file("examples/data/xgxr2.rds", package="NMdata"))
dt.flags <- data.frame(
  flagn=10,
  flagc="Below LLOQ",
  condition=c("BLQ==1")
)
pk <- flagsAssign(pk, dt.flags, subset.data="EVID==0", col.flagn="flagn", col.flagc="flagc")
pk <- flagsAssign(pk, subset.data="EVID==1", flagc.0="Dosing",
  col.flagn="flagn", col.flagc="flagc")
unique(pk[, c("EVID", "flagn", "flagc", "BLQ")])
flagsCount(pk[EVID==0], dt.flags, col.flagn="flagn", col.flagc="flagc")
```

 fnExtension

Change file name extension

Description

Very simple but often applicable function to change the file name extension (from say file.lst to file.mod)

Usage

```
fnExtension(fn, ext)
```

Arguments

fn	file name
ext	new file name extension

Value

A text string

Examples

```
fnExtension("file.lst", ".mod")
fnExtension("file.lst", "")
```

is.NMdata	<i>Check if an object is 'NMdata'</i>
-----------	---------------------------------------

Description

Check if an object is 'NMdata'

Usage

```
is.NMdata(x)
```

Arguments

x Any object

Value

logical if x is an 'NMdata' object

listMissings	<i>List rows with missing values across multiple columns</i>
--------------	--

Description

Missing can be NA and for character variables it can be certain strings too. This function is experimental and design may change in future releases.

Usage

```
listMissings(data, cols, by, na.strings = c("", "."), quiet = FALSE, as.fun)
```

Arguments

data	The data to look into.
cols	The columns to look for missings in.
by	If supplied, we are keeping track of the missings within the values of the by columns. In summary, by is included too.
na.strings	Strings that should be interpreted as missing. All spaces will be removed before we compare to na.strings. The default is c("", ".") so say " ." is a missing by default.

quiet	Keep quiet? Default is not to.
as.fun	A function that will be run on the result before returning. If first input data set is a data.table, the default is to return a data.table, if not the default is to return a data.frame. Use whatever to get what fits in with your workflow. Default can be configured with NMdataConf.

See Also

Other DataWrangling: [compareCols\(\)](#), [dims\(\)](#)

mergeCheck	<i>Merge, order, and check resulting rows and columns.</i>
------------	--

Description

Stop checking that the number of rows is unchanged after a merge - mergeCheck checks what you really want - i.e. x is extended with columns from y while all rows in x are retained, and no new rows are created (plus some more checks). mergeCheck is not a merge implementation - it is a useful merge wrapper. The advantage over using much more flexible merge or join function lies in the fully automated checking that the results are consistent with the simple merge described above.

Usage

```
mergeCheck(
  x,
  y,
  by,
  by.x,
  by.y,
  fun.commoncols = base::warning,
  ncols.expect,
  track.msg = FALSE,
  quiet,
  df1,
  df2,
  fun.na.by = base::stop,
  as.fun,
  ...
)
```

Arguments

x	A data.frame with the number of rows must should be obtained from the merge. The resulting data.frame will be ordered like x.
y	A data.frame that will be merged onto x.
by	The column(s) to merge by. Character string (vector). by or by.x and by.y must be supplied.

<code>by.x</code>	If the columns to merge by in <code>x</code> and <code>y</code> are named differently. <code>by</code> or <code>by.x</code> and <code>by.y</code> must be supplied.
<code>by.y</code>	If the columns to merge by in <code>x</code> and <code>y</code> are named differently. <code>by</code> or <code>by.x</code> and <code>by.y</code> must be supplied.
<code>fun.commoncols</code>	If common columns are found in <code>x</code> and <code>y</code> , and they are not used in <code>by</code> , this will create columns named like <code>col.x</code> and <code>col.y</code> in result (see <code>?merge</code>). Often, this is a mistake, and the default is to throw a warning if this happens. If using <code>mergeCheck</code> in a function, you may want to make sure this is not happening and use <code>fun.commoncols=stop</code> . If you want nothing to happen, you can do <code>fun.commoncols=NULL</code> .
<code>ncols.expect</code>	If you want to include a check of the number of columns being added to the dimensions of <code>x</code> . So if <code>ncols.expect=1</code> , the resulting data must have exactly one column more than <code>x</code> - if not, an error will be returned.
<code>track.msg</code>	If using <code>mergeCheck</code> inside other functions, it can be useful to use <code>track.msg=TRUE</code> . This will add information to messages/warnings/errors that they came from <code>mergeCheck</code> .
<code>quiet</code>	If <code>FALSE</code> , the names of the added columns are reported. Default value controlled by <code>NMdataConf</code> .
<code>df1</code>	Deprecated. Use <code>x</code> .
<code>df2</code>	Deprecated. Use <code>y</code> .
<code>fun.na.by</code>	If NA's are found in (matched) by columns in both <code>x</code> and <code>y</code> , what should we do? This could be OK, but in many cases, it's because something unexpected is happening. Use <code>fun.na.by=NULL</code> in cases where you really don't care about this and want to go ahead regardless.
<code>as.fun</code>	The default is to return a <code>data.table</code> if <code>x</code> is a <code>data.table</code> and return a <code>data.frame</code> in all other cases. Pass a function in <code>as.fun</code> to convert to something else.
<code>...</code>	additional arguments passed to <code>data.table::merge</code> . If all is among them, an error will be returned.

Details

Besides merging and checking rows, `mergeCheck` makes sure the order in `x` is retained in the resulting data (both rows and column order). Also, a warning is given if column names are overlapping, making `merge` create new column names like `col.x` and `col.y`. Merges and other operations are done using `data.table`. If `x` is a `data.frame` (and not a `data.table`), it will internally be converted to a `data.table`, and the resulting `data.table` will be converted back to a `data.frame` before returning.

`mergeCheck` is for the kind of merges where we think of `x` as the data to be enriched with columns from `y` - rows unchanged. This is even further limited than a left join where you can match rows multiple times. A common example of the use of `mergeCheck` is for adding covariates to a `pk/pd` data set. We do not want that to remove or duplicate doses, observations, or simulation records. In those cases, `mergeCheck` does all needed checks, and you can run full speed without checking dimensions (which is anyway not exactly the right thing to do in the general case) or worry that something might go wrong.

Checks performed:

- `x` has `>0` rows

- by columns are present in x and y
- Merge is not performed on NA values. If by=ID and both x\$ID and y\$ID contain NA's, an error is thrown (see argument fun.na.by).
- Merge is done by all common column names in x and y. A warning is thrown if there are column names that are not being used to merge by. This will result in two columns named like BW.x and BW.y and is often unintended.
- Before merging a row counter is added to x. After the merge, the result is assured to have exactly one occurrence of each of the values of the row counter in x.

Moreover, row and column order from x is retained in the result.

Value

a data.frame resulting from merging x and y. Class as defined by as.fun.

See Also

Other DataCreate: [NMorderColumns\(\)](#), [NMstamp\(\)](#), [findCovs\(\)](#), [findVars\(\)](#), [flagsAssign\(\)](#), [flagsCount\(\)](#), [tmpcol\(\)](#)

Examples

```
df1 <- data.frame(x = 1:10,
                 y=letters[1:10],
                 stringsAsFactors=FALSE)
df2 <- data.frame(y=letters[1:11],
                 x2 = 1:11,
                 stringsAsFactors=FALSE)

mc1 <- mergeCheck(df1,df2,by="y")

## Notice as opposed to most merge/join algorithms, mergeCheck by
## default retains both row and column order from x
library(data.table)
merge(as.data.table(df1),as.data.table(df2))
## Here we get a duplicate of a df1 row in the result. If we only
## check dimensions, we make a mistake. mergeCheck captures the
## error - and tell us where to find the problem (ID 31 and 180):
## Not run:
pk <- readRDS(file=system.file("examples/data/xgxr2.rds",package="NMdata"))
dt.cov <- pk[,.(ID=unique(ID))]
dt.cov[,COV:=sample(1:5,size=.N,replace=TRUE)]
dt.cov <- dt.cov[c(1,1:(.N-1))]
dim(pk)
res.merge <- merge(pk,dt.cov,by="ID")
dim(res.merge)
mergeCheck(pk,dt.cov,by="ID")

## End(Not run)
```

NMcheckColnames	<i>Compare \$INPUT in control stream to column names in input data</i>
-----------------	--

Description

Misspecification of column names in \$DATA are a common source of problems with Nonmem models, and one of the first things to check when seemingly inexplicable things happen. This function lines up input data column names with \$DATA and how NMscanData will interpret \$DATA so you can easily spot if something is off.

Usage

```
NMcheckColnames(file, as.fun, ...)
```

Arguments

file	A Nonmem control stream or list file
as.fun	See ?NMdataConf
...	Additional arguments passed to

Value

An overview of input column names and how they are translated

NMcheckData	<i>Check data for Nonmem compatibility</i>
-------------	--

Description

Check data in various ways for compatibility with Nonmem. Some findings will be reported even if they will not make Nonmem fail but because they are typical dataset issues.

Usage

```
NMcheckData(
  data,
  file,
  covs,
  covs.occ,
  cols.num,
  col.id = "ID",
  col.time = "TIME",
  col.cmt = "CMT",
  col.flagn,
  col.row,
```

```

na.strings,
return.summary = FALSE,
quiet = FALSE,
as.fun
)

```

Arguments

<code>data</code>	The data to check. <code>data.frame</code> , <code>data.table</code> , <code>tibble</code> , anything that can be converted to <code>data.table</code> .
<code>file</code>	Alternatively to checking a data object, you can use <code>file</code> to specify a control stream to check. This can either be a (working or non-working) input control stream or an output control stream. In this case, <code>NMdataCheck</code> checks column names in <code>data</code> against control stream (see <code>NMcheckColnames</code>), reads the data as <code>NONMEM</code> would do, and do the same checks on the data as <code>NMdataCheck</code> would do using the <code>data</code> argument. <code>col.flagn</code> is ignored in this case - instead, <code>ACCEPT/IGNORE</code> statements in control stream are applied. The <code>file</code> argument is useful for debugging a <code>Nonmem</code> model.
<code>covs</code>	columns that contain subject-level covariates. They are expected to be non-missing, numeric and not varying within subjects.
<code>covs.occ</code>	A list specifying columns that contain subject:occasion-level covariates. They are expected to be non-missing, numeric and not varying within combinations of subject and occasion. <code>covs.occ=list(PERIOD=c("FED"))</code> means that <code>FED</code> is the covariate, while <code>PERIOD</code> indicates the occasion.
<code>cols.num</code>	Columns that are expected to be present, numeric and non-NA. If a character vector is given, the columns are expected to be used in all rows. If a column is only used for a subset of rows, use a list and name the elements by subsetting strings. See examples.
<code>col.id</code>	The name of the column that holds the subject identifier. Default is "ID".
<code>col.time</code>	The name of the column holding actual time.
<code>col.cmt</code>	The name(s) of the compartment column(s). These will be checked to be positive integers for all rows. They are also used in checks for row duplicates.
<code>col.flagn</code>	Optionally, the name of the column holding numeric exclusion flags. Default value is <code>FLAG</code> and can be configured using <code>NMdataConf</code> . Disable by using <code>col.flagn=FALSE</code> .
<code>col.row</code>	A column with a unique value for each row. Such a column is recommended to use if possible. Default ("ROW") can be modified using <code>NMdataConf</code> .
<code>na.strings</code>	Strings to be accepted when trying to convert characters to numerics. This will typically be a string that represents missing values. Default is "." even though most users will use actual NA (<code>NA_character</code>), i.e. not a string. See <code>?NMisNumeric</code> .
<code>return.summary</code>	If <code>TRUE</code> (not default), the table summary that is printed if <code>quiet=FALSE</code> is returned as well. In that case, a list is returned, and the findings are in an element called <code>findings</code> .
<code>quiet</code>	Keep quiet? Default is not to.

`as.fun` The default is to return data as a `data.frame`. Pass a function (say `tibble::as_tibble`) in `as.fun` to convert to something else. If `data.tables` are wanted, use `as.fun="data.table"`. The default can be configured using `NMdataConf`.

Details

The following checks are performed. The term "numeric" does not refer to a numeric representation in R, but compatibility with Nonmem. The character string "2" is in this sense a valid numeric, "id2" is not.

- Column names must be unique and not contain special characters
- If an exclusion flag is used (for ACCEPT/IGNORE in Nonmem), elements must be non-missing and integers. If an exclusion flag is found, the rest of the checks are performed on rows where that flag equals 0 (zero) only.
- If a unique row identifier is found, it has to be non-missing, increasing integers.
- `col.time` (TIME), EVID, ID, CMT, MDV: If present, elements must be non-missing and numeric.
- `col.time` (TIME) must be non-negative
- EVID must be in 0,1,2,3,4
- CMT must be positive integers. However, can be missing or zero for EVID==3.
- MDV must be the binary (1/0) representation of `is.na(DV)`
- AMT must be 0 or NA for EVID 0 and 2
- AMT must be positive for EVID 1 and 4
- DV must be numeric
- DV must be missing for EVID in 1,4.
- If found, RATE must be a numeric, equaling -2 or non-negative for dosing events.
- If found, SS must be a numeric, equaling 0 or 1 for dosing records.
- If found, ADDL must be a non-negative integer for dosing records. II must be present.
- If found, II must be a non-negative integer for dosing records. ADDL must be present.
- ID must be positive and values cannot be disjoint (all records for each ID must be following each other. This is technically not a requirement in Nonmem but most often an error. Use a second ID column if you deliberately want to soften this check)
- TIME cannot be decreasing within ID, unless EVID in 3,4.
- all ID's must have doses (EVID in 1,4)
- all ID's must have observations (EVID==0)
- If a unique row identifier is used, this must be non-missing, increasing, integer
- Character values must not contain commas (they will mess up writing/reading csv)
- Columns specified in `covs` argument must be non-missing, numeric and not varying within subjects.
- Columns specified in `covs.occ` must be non-missing, numeric and not varying within combinations of subject and occasion.
- Columns specified in `cols.num` must be present, numeric and non-NA.

Examples

```
dat <- readRDS(system.file("examples/data/xgxr2.rds", package="NMdata"))
NMcheckData(dat)
dat[EVID==0, LLOQ:=3.5]
## expecting LLOQ only for samples
NMcheckData(dat, cols.num=list(c("STUDY"), "EVID==0"=c("LLOQ")))
```

NMdataConf

Configure default behavior of NMdata functions

Description

Configure default behavior across the functions in NMdata rather than typing the arguments in all function calls. Configure for your file organization, data set column names, and other NMdata behaviour. Also, you can control what data class NMdata functions return (say data.tables or tibbles if you prefer one of those over data.frames).

Usage

```
NMdataConf(...)
```

Arguments

...

NMdata options to modify. These are named arguments, like for base::options. Normally, multiple arguments can be used. The exception is if reset=TRUE is used which means all options are restored to default values. If NULL is passed to an argument, the argument is reset to default. See examples for how to use. Parameters that can be controlled are:

- `args.fread` Arguments passed to fread when reading `_input_` data files (fread options for reading Nonmem output tables cannot be configured at this point). If you change this, you are starting from scratch, except from file. This means that existing default argument values are all disregarded.
- `args.fwrite` Arguments passed to fwrite when writing csv files (NMwriteData). If you use this, you have to supply all arguments you want to use with fwrite, except for `x` (the data) and file.
- `as.fun` A function that will be applied to data returned by various data reading functions (NMscanData, NMreadTab, NMreadCsv, NMscanInput, NMscanTables). Also, data processing functions like mergeCheck, findCovs, findVars, flagsAssign, flagsCount take this into account, but slightly differently. For these functions that take data as arguments, the `as.fun` configuration is only taken into account if the data passed to the functions are not of class `data.table`. The argument `as.fun` to these functions is always adhered to. Pass an actual function, say `as.fun=tibble::as_tibble`. If you want `data.table`, use `as.fun="data.table"` (not a function).

- `check.time` Logical, applies to `NMscanData` only. `NMscanData` by default checks if output control stream is newer than input control stream and input data. Set this to `FALSE` if you are in an environment where time stamps cannot be relied on.
- `col.flagc` The name of the column containing the character flag values for data row omission. Default value is `flag`. Used by `flagsAssign`, `flagsCount`.
- `col.flagn` The name of the column containing numerical flag values for data row omission. Default value is `FLAG`. Used by `flagsAssign`, `flagsCount`, `NMcheckData`.
- `col.model` The name of the column that will hold the name of the model. See `modelname` too (which defines the values that the column will hold).
- `col.nmout` A column of this name will be a logical representing whether row was in output table or not.
- `col.nomtime` The name of the column holding nominal time. This is only used for sorting columns by `NMorderColumns`.
- `col.row` The name of the column containing a unique row identifier. This is used by `NMscanData` when `merge.by.row=TRUE`, and by `NMorderColumns` (row counter will be first column in data).
- `file.mod` A function that will derive the path to the input control stream based on the path to the output control stream. Technically, it can be a string too, but when using `NMdataConf`, this would make little sense because it would direct all output control streams to the same input control streams.
- `merge.by.row` Adjust the default combine method in `NMscanData`.
- `modelname` A function that will translate the output control stream path to a model name. Default is to strip `.lst`, so `/path/to/run1.lst` will become `run1`. Technically, it can be a string too, but when using `NMdataConf`, this would make little sense because it would translate all output control streams model name.
- `quiet` For non-interactive scripts, you can switch off the chatty behavior once and for all using this setting.
- `recover.rows` In `NMscanData`, Include rows from input data files that do not exist in output tables? This will be added to the `$row` dataset only, and `$run`, `$id`, and `$occ` datasets are created before this is taken into account. A column called `nmout` will be `TRUE` when the row was found in output tables, and `FALSE` when not. Default is `FALSE`.
- `use.input` In `NMscanData`, merge with columns in input data? Using this, you don't have to worry about remembering including all relevant variables in the output tables. Default is `TRUE`.
- `use.rds` Affects `NMscanData` and `NMscanInput`.

Details

Recommendation: Use this function transparently in the code and not in a configuration file hidden from other users.

Value

If no arguments given, a list of active settings. If arguments given and no issues found, TRUE invisibly.

Examples

```
## get current defaults
NMdataConf()
## change a parameter
NMdataConf(check.time=FALSE)
## reset one parameter to default value
NMdataConf(modelname=NULL)
## reset all parameters to defaults
NMdataConf(reset=TRUE)
```

NMdataOperations	<i>Basic arithmetic</i>
------------------	-------------------------

Description

Basic arithmetic

Usage

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

## S3 method for class 'NMdata'
t(x, ...)

## S3 method for class 'NMdata'
dimnames(x, ...)

## S3 method for class 'NMdata'
rbind(x, ...)

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

Arguments

x	an NMdata object
...	arguments passed to other methods.

Details

When 'dimnames', 'merge', 'cbind', 'rbind', or 't' is called on an 'NMdata' object, the 'NMdata' class is dropped, and then the operation is performed. So if an 'NMdata' object inherits from 'data.frame' and no other classes (which is default), these operations will be performed using the 'data.frame' methods. But for example, if you use 'as.fun' to get a 'data.table' or 'tbl', their respective methods are used instead.

Value

An object that is not of class 'NMdata'.

NMextractDataFile	<i>Extract the data file used in a control stream</i>
-------------------	---

Description

Extract the data file used in a control stream

Usage

```
NMextractDataFile(file, dir.data = NULL, file.mod)
```

Arguments

file	The input control stream or the list file.
dir.data	See NMscanInput. If used, only the file name mentioned in \$DATA is used. dir.data will be used as the path, and the existence of the file in that directory is not checked.
file.mod	The input control stream. Default is to look for "file" with extension changed to .mod (PSN style). You can also supply the path to the file, or you can provide a function that translates the output file path to the input file path. The default behavior can be configured using NMdataConf. See dir.data too.

Value

The path to the input data file.

NMextractText	<i>Versatile text extractor from Nonmem (input or output) control streams</i>
---------------	---

Description

If you want to extract input sections like \$PROBLEM, \$DATA etc, see NMreadSection. This function is more general and can be used to extract eg result sections.

Usage

```

NMextractText(
  file,
  lines,
  text,
  section,
  char.section,
  char.end = char.section,
  return = "text",
  keepEmpty = FALSE,
  keepName = TRUE,
  keepComments = TRUE,
  asOne = TRUE,
  simplify = TRUE,
  cleanSpaces = FALSE,
  type = "mod",
  linesep = "\n"
)

```

Arguments

file	A file path to read from. Normally a .mod or .lst. See lines and text as well.
lines	Text lines to process. This is an alternative to using the file and text arguments.
text	Use this argument if the text to process is one long character string, and indicate the line separator with the linesep argument. Use only one of file, lines, and text.
section	The name of section to extract. Examples: "INPUT", "PK", "TABLE", etc. It can also be result sections like "MINIMIZATION".
char.section	The section denoter as a string compatible with regular expressions. "\$" for sections in .mod files, "0" for results in .lst files.
char.end	A regular expression to capture the end of the section. The default is to look for the next occurrence of char.section.
return	If "text", plain text lines are returned. If "idx", matching line numbers are returned. "text" is default.
keepEmpty	Keep empty lines in output? Default is FALSE.
keepName	Keep the section name in output (say, "\$PROBLEM") Default is TRUE. It can only be FALSE, if return"idx".

keepComments	Keep comment lines?
asOne	If multiple hits, concatenate into one. This will most often be relevant with name="TABLE". If FALSE, a list will be returned, each element representing a table. Default is TRUE. So if you want to process the tables separately, you probably want FALSE here.
simplify	If asOne=FALSE, do you want the result to be simplified if only one table is found? Default is TRUE which is desirable for interactive analysis. For programming, you probably want FALSE.
cleanSpaces	If TRUE, leading and trailing are removed, and multiplied succeeding white spaces are reduced to single white spaces.
type	Either mod, res or NULL. mod is for information that is given in .mod (.lst file can be used but results section is disregarded). If NULL, NA or empty string, everything is considered.
linesep	If using the text argument, use linesep to indicate how lines should be separated.

Details

This function is planned to get a more general name and then be called by NMreadSection.

Value

character vector with extracted lines.

See Also

Other Nonmem: [NMapplyFilters\(\)](#), [NMgenText\(\)](#), [NMreadSection\(\)](#), [NMwriteData\(\)](#), [NMwriteSection\(\)](#)

Examples

```
NMreadSection(system.file("examples/nonmem/xgxr001.lst", package = "NMdata"), section="DATA")
```

NMgenText	<i>Generate text for INPUT and possibly DATA sections of NONMEM control streams.</i>
-----------	--

Description

The user is provided with text to use in Nonmem. NMwriteSection can use the results to update the control streams. INPUT lists names of the data columns while DATA provides a path to data and ACCEPT/IGNORE statements. Once a column is reached that Nonmem will not be able to read as a numeric and column is not in nm.drop, the list is stopped. Only exception is TIME which is not tested for whether character or not.

Usage

```

NMgenText(
  data,
  drop,
  col.flagn = "FLAG",
  rename,
  copy,
  file,
  dir.data,
  capitalize = FALSE,
  allow.char.TIME = TRUE,
  quiet
)

```

Arguments

data	The data that NONMEM will read.
drop	Only used for generation of proposed text for INPUT section. Columns to drop in Nonmem \$INPUT. This has two implications. One is that the proposed \$INPUT indicates =DROP after the given column names. The other that in case it is a non-numeric column, succeeding columns will still be included in \$INPUT and can be read by NONMEM.
col.flagn	Name of a numeric column with zero value for rows to include in Nonmem run, non-zero for rows to skip. The argument is only used for generating the proposed \$DATA text to paste into the Nonmem control stream. To skip this feature, use col.flagn=NULL. Default is defined by NMdataConf.
rename	For the \$INPUT text proposal only. If you want to rename columns in NONMEM \$DATA, NMwriteData can adjust the suggested \$DATA text. If you plan to use BBW instead of BWBASE in Nonmem, consider nm.rename=c(BBW="BWBASE"). The result will include BBW and not BWBASE.
copy	For the \$INPUT text proposal only. If you plan to use additional names for columns in Nonmem \$INPUT, NMwriteData can adjust the suggested \$INPUT text. Say you plan to use CONC as DV in Nonmem, use rename=c(DV="CONC"), i.e. rename=c(newname="existing"). INPUT suggestion will in this case contain DV=CONC.
file	The file name NONMEM will read the data from (for the \$DATA section). It can be a full path.
dir.data	For the \$DATA text proposal only. The path to the input datafile to be used in the Nonmem \$DATA section. Often, a relative path to the actual Nonmem run is wanted here. If this is used, only the file name and not the path from the file argument is used.
capitalize	For the \$INPUT text proposal only. If TRUE, all column names in \$INPUT text will be converted to capital letters.
allow.char.TIME	For the \$INPUT text proposal only. Assume Nonmem can read TIME even if it can't be translated to numeric. This is necessary if using the 00:00 format. Default is TRUE.

quiet Hold messages back? Default is defined by NMdataConf.

Value

Text for inclusion in Nonmem control stream, invisibly.

See Also

Other Nonmem: [NMapplyFilters\(\)](#), [NMextractText\(\)](#), [NMreadSection\(\)](#), [NMwriteData\(\)](#), [NMwriteSection\(\)](#)

NMinfo *Get metadata from an NMdata object*

Description

Extract metadata such as info on tables, columns and further details in your favorite class

Usage

```
NMinfo(data, info, as.fun)
```

Arguments

data	An object of class NMdata (a result of NMscanData)
info	If not passed, all the metadata is returned. You can use "details", "tables", or "columns" to get only these subsets. If info is "tables" or "columns"
as.fun	The default is to return data as a data.frame. Pass a function (say <code>tibble::as_tibble</code>) in as.fun to convert to something else. If data.tables are wanted, use <code>as.fun="data.table"</code> . The default can be configured using NMdataConf.

Value

A table of class as defined by as.fun in case info is "columns" or "tables". A list if info missing or equal to "details".

NMisNumeric	<i>Test if a variable can be interpreted by Nonmem</i>
-------------	--

Description

Nonmem can only interpret numeric data. However, a factor or a character variable may very well be interpretable by Nonmem (e.g. "33"). This function tells whether Nonmem will be able to read it.

Usage

```
NMisNumeric(x, na.strings = ".", each = FALSE)
```

Arguments

x	The vector to check Don't export
na.strings	Tolerated strings that do not translate to numerics. Default is to accept "." because it's common to write missing values that way to Nonmem (even if Nonmem will handle them as zeros rather than missing). Notice actual NA's are accepted so you may want to use na.strings=NULL if you don't code missings as "." and just do this when writing the data set to a delimited file (like NMwriteData will do for you).
each	Use each=TRUE to evaluate each element in a vector individually. The default is to return a single-length logical for a vector x summarizing whether all the elements are numeric-compatible.

Value

TRUE or FALSE

NMorderColumns	<i>Standardize column order in Nonmem input data</i>
----------------	--

Description

Order data columns for easy export to Nonmem. No data values are edited. The order is configurable through multiple arguments. See details.

Usage

```

NMorderColumns(
  data,
  first,
  last,
  lower.last = FALSE,
  chars.last = TRUE,
  alpha = TRUE,
  col.nomtime,
  col.row,
  col.flagn,
  col.dv = "DV",
  as.fun = NULL,
  quiet
)

```

Arguments

<code>data</code>	The dataset which columns to reorder.
<code>first</code>	Columns that should come almost first. See details.
<code>last</code>	Columns to move to back of dataset. If you work with a large dataset, and some columns are irrelevant for the Nonmem runs, you can use this argument.
<code>lower.last</code>	Should columns which names contain lowercase characters be moved towards the back? Some people use a standard of lowercase variables (say "race") being character representations ("asian", "caucasian", etc.) variables and the uppercase (1,2,...) being the numeric representation for Nonmem.
<code>chars.last</code>	Should columns which cannot be converted to numeric be put towards the end? A column can be a character or a factor in R, but still be valid in Nonmem (often the case for ID which can only contain numeric digits but really is a character or factor). So rather than only looking at the column class, the columns are attempted converted to numeric. Notice, it will attempted to be converted to numeric to test whether Nonmem will be able to make sense of it, but the values in the resulting dataset will be untouched. No values will be edited. If TRUE, logicals will always be put last. NA's must be NA or ".".
<code>alpha</code>	Sort columns alphabetically. Notice, this is the last order priority applied.
<code>col.nomtime</code>	The name of the column containing nominal time. If given, it will put the column quite far left, just after row counter and ID. Default value is NOMTIME and can be configured with NMdataConf.
<code>col.row</code>	A row counter column. This will be the first column in the dataset. Technically, you can use it for whatever column you want first. Default value is ROW and can be configured with NMdataConf.
<code>col.flagn</code>	The name of the column containing numerical flag values for data row omission. Default value is FLAG and can be configured with NMdataConf.
<code>col.dv</code>	a vector of column names to put early to represent dependent variable(s). Default is DV.

as.fun	The default is to return a data.table if data is a data.table and return a data.frame in all other cases. Pass a function in as.fun to convert to something else. The default can be configured using NMdataConf. However, if data is a data.table, settings via NMdataConf are ignored.
quiet	If true, no warning will be given about missing standard Nonmem columns.

Details

This function will change the order of columns but it will never edit values in any columns. The ordering is by the following steps, each step depending on corresponding argument.

- "col.row - "Row id if argument row is non-NULL
- "not editable - "ID (if a column is called ID)
- "col.ntime - "Nominal time.
- "first - "user-specified first columns
- "not editable - "Standard Nonmem columns: TIME, EVID, CMT, AMT, RATE, DV, MDV
- "last - "user-specified last columns
- "chars.last - "numeric, or interpretable as numeric
- "not editable - "less often used nonmem names: col.flagn, OCC, ROUTE, GRP, TRIAL, DRUG, STUDY
- "lower.last - "lower case in name
- "alpha - "Alphabetic/numeric sorting

Value

data with modified column order.

See Also

Other DataCreate: [NMstamp\(\)](#), [findCovs\(\)](#), [findVars\(\)](#), [flagsAssign\(\)](#), [flagsCount\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

NMreadCsv

Read input data formatted for nonmem

Description

This function is especially useful if the csv file was written using NMwriteData.

Usage

```
NMreadCsv(file, args.fread, as.fun = NULL)
```

Arguments

file	The file to read. Must be pure text.
args.fread	List of arguments passed to fread. Notice that except for "file", you need to supply all arguments to fread if you use this argument. Default values can be configured using NMdataConf.
as.fun	The default is to return data as a data.frame. Pass a function (say tibble::as_tibble) in as.fun to convert to something else. If data.tables are wanted, use as.fun="data.table". The default can be configured using NMdataConf.

Details

This is almost just a shortcut to fread so you don't have to remember how to read the data that was exported for nonmem. The only added feature is that meta data as written by NMwriteData is read and attached as NMdata metadata before data is returned.

Value

A data set of class as defined by as.fun.

See Also

NMwriteData

Other DataRead: [NMreadTab\(\)](#), [NMscanData\(\)](#), [NMscanInput\(\)](#), [NMscanTables\(\)](#)

NMreadSection

Extract sections of Nonmem control streams

Description

This is a very commonly used wrapper for the input part of the model file. Look NMextractText for more general functionality suitable for the results part too.

Usage

```
NMreadSection(  
  file = NULL,  
  lines = NULL,  
  text = NULL,  
  section,  
  return = "text",  
  keepEmpty = FALSE,  
  keepName = TRUE,  
  keepComments = TRUE,  
  asOne = TRUE,  
  simplify = TRUE,  
  cleanSpaces = FALSE,
```

```

    ...
)

NMgetSection(...)

```

Arguments

file	A file path to read from. Normally a .mod or .lst. See lines also.
lines	Text lines to process. This is an alternative to using the file argument.
text	Use this argument if the text to process is one long character string, and indicate the line separator with the linesep argument (handled by NMextractText). Use only one of file, lines, and text.
section	The name of section to extract without "\$". Examples: "INPUT", "PK", "TABLE", etc. Not case sensitive.
return	If "text", plain text lines are returned. If "idx", matching line numbers are returned. "text" is default.
keepEmpty	Keep empty lines in output? Default is FALSE.
keepName	Keep the section name in output (say, "\$PROBLEM") Default is TRUE. It can only be FALSE, if return"idx".
keepComments	Keep comment lines?
asOne	If multiple hits, concatenate into one. This will most often be relevant with name="TABLE". If FALSE, a list will be returned, each element representing a table. Default is TRUE. So if you want to process the tables separately, you probably want FALSE here.
simplify	If asOne=FALSE, do you want the result to be simplified if only one section is found? Default is TRUE which is desirable for interactive analysis. For programming, you probably want FALSE.
cleanSpaces	If TRUE, leading and trailing are removed, and multiplied succeeding white spaces are reduced to single white spaces.
...	Additional arguments passed to NMextractText

Value

character vector with extracted lines.

Functions

- NMgetSection: Old function name for NMreadSection

See Also

Other Nonmem: [NMapplyFilters\(\)](#), [NMextractText\(\)](#), [NMgenText\(\)](#), [NMwriteData\(\)](#), [NMwriteSection\(\)](#)

Examples

```
NMreadSection(system.file("examples/nonmem/xgxr001.lst", package="NMdata"), section="DATA")
```

NMreadTab	<i>Read an output table file from NONMEM</i>
-----------	--

Description

Read a table generated by a \$TABLE statement in Nonmem. Generally, these files cannot be read by read.table or similar because formatting depends on options in the \$TABLE statement, and because Nonmem sometimes includes extra lines in the output that have to be filtered out. NMreadTab can do this automatically based on the table file alone.

Usage

```
NMreadTab(file, tab.count = TRUE, quiet, as.fun, ...)
```

Arguments

file	path to NONMEM table file
tab.count	Nonmem includes a counter of tables in the written data files. These are often not useful. However, if tab.count is TRUE (default), a counter of tables is included as a column called TABLENO. Just notice, the table numbers in TABLENO are just cumulatively counting the number of tables reported in the file. TABLENO is not true to the actual table number as given by Nonmem.
quiet	logical stating whether or not information is printed about what is being done. Default can be configured using NMdataConf.
as.fun	The default is to return data as a data.frame. Pass a function (say tibble::as_tibble) in as.fun to convert to something else. If data.tables are wanted, use as.fun="data.table". The default can be configured using NMdataConf.
...	Arguments passed to fread.

Details

The actual reading of data is based on data.table::fread. Generally, the function is fast thanks to data.table.

Value

The Nonmem table data.

See Also

Other DataRead: [NMreadCsv\(\)](#), [NMscanData\(\)](#), [NMscanInput\(\)](#), [NMscanTables\(\)](#)

 NMscanData

Automatically find Nonmem input and output tables and organize data

Description

This is a very general solution to automatically identifying, reading, and merging all output and input data in a Nonmem model. The most important steps are

- Read and combine output tables,
- If wanted, read input data and restore variables that were not output from the nonmem model
- If wanted, also restore rows from input data that were disregarded in Nonmem (e.g. observations or subjects that are not part of the analysis)

Usage

```

NMscanData(
  file,
  col.row,
  use.input,
  merge.by.row,
  recover.rows,
  file.mod,
  dir.data,
  translate.input = TRUE,
  quiet,
  use.rds,
  args.fread,
  as.fun,
  col.id = "ID",
  modelname,
  col.model,
  col.nmout,
  tab.count = FALSE,
  order.columns = TRUE,
  check.time
)

```

Arguments

<code>file</code>	A nonmem control stream or output file from nonmem (.mod or .lst)
<code>col.row</code>	A column with a unique value for each row. Such a column is recommended to use if possible. See <code>merge.by.row</code> and details as well. Default ("ROW") can be modified using <code>NMdataConf</code> .
<code>use.input</code>	Should the input data be added to the output data. Only column names that are not found in output data will be retrieved from the input data. Default is TRUE which can be modified using <code>NMdataConf</code> . See <code>merge.by.row</code> too.

<code>merge.by.row</code>	If <code>use.input=TRUE</code> , this argument determines the method by which the input data is added to output data. The default method (<code>merge.by.row=FALSE</code>) is to interpret the Nonmem code to immitate the data filtering (IGNORE and ACCEPT statements), but the recommended method is <code>merge.by.row=TRUE</code> which means that data will be merged by a unique row identifier. The row identifier must be present in input and at least one full length output data table. See argument <code>col.row</code> too.
<code>recover.rows</code>	Include rows from input data files that do not exist in output tables? This will be added to the <code>\$row</code> dataset only, and <code>\$run</code> , <code>\$id</code> , and <code>\$occ</code> datasets are created before this is taken into account. A column called <code>nmout</code> will be <code>TRUE</code> when the row was found in output tables, and <code>FALSE</code> when not. Default is <code>FALSE</code> and can be configured using <code>NMdataConf</code> .
<code>file.mod</code>	The input control stream. Default is to look for <code>"file"</code> with extension changed to <code>.mod</code> (PSN style). You can also supply the path to the file, or you can provide a function that translates the output file path to the input file path. The default behavior can be configured using <code>NMdataConf</code> . See <code>dir.data</code> too.
<code>dir.data</code>	The data directory can only be read from the control stream (<code>.mod</code>) and not from the output file (<code>.lst</code>). So if you only have the output control stream, use <code>dir.data</code> to tell in which directory to find the data file. If <code>dir.data</code> is provided, the <code>.mod</code> file is not used at all.
<code>translate.input</code>	Default is <code>TRUE</code> , meaning that input data column names are translated according to <code>\$INPUT</code> section in nonmem listing file.
<code>quiet</code>	The default is to give some information along the way on what data is found. But consider setting this to <code>TRUE</code> for non-interactive use. Default can be configured using <code>NMdataConf</code> .
<code>use.rds</code>	If an <code>rds</code> file is found with the exact same name (except for <code>.rds</code> instead of say <code>.csv</code>) as the input data file mentioned in the Nonmem control stream, should this be used instead? The default is yes, and <code>NMwriteData</code> will create this by default too. Default can be configured using <code>NMdataConf</code> .
<code>args.fread</code>	List of arguments passed to when reading <code>_input_</code> data. Notice that except for "input" and "file", you need to supply all arguments to <code>fread</code> if you use this argument. Default values can be configured using <code>NMdataConf</code> .
<code>as.fun</code>	The default is to return data as a <code>data.frame</code> . Pass a function (say <code>tibble::as_tibble</code>) in <code>as.fun</code> to convert to something else. If <code>data.tables</code> are wanted, use <code>as.fun="data.table"</code> . The default can be configured using <code>NMdataConf</code> .
<code>col.id</code>	The name of the subject ID variable, default is "ID".
<code>modelName</code>	The model name to be stored if <code>col.model</code> is not <code>NULL</code> . If not supplied, the name will be taken from the control stream file name by omitting the directory/path and deleting the <code>.lst</code> extension (<code>path/run001.lst</code> becomes <code>run001</code>). This can be a character string or a function which is called on the value of <code>file</code> (<code>file</code> is another argument to <code>NMscanData</code>). The function must take one character argument and return another character string. As example, see <code>NMdataConf()\$modelName</code> . The default can be configured using <code>NMdataConf</code> .

<code>col.model</code>	A column of this name containing the model name will be included in the returned data. The default is to store this in a column called "model". See argument "modelname" as well. Set to NULL if not wanted. Default can be configured using NMdataConf.
<code>col.nmout</code>	A column of this name will be a logical representing whether row was in output table or not. Default can be modified using NMdataConf.
<code>tab.count</code>	Nonmem includes a counter of tables in the written data files. These are often not useful. Especially for NMscanData output it can be meaningless because multiple tables can be combined so this information is not unique across those source tables. However, if <code>tab.count</code> is TRUE (not default), this will be carried forward and added as a column called TABLENO. The argument is passed to NMscanTables.
<code>order.columns</code>	If TRUE (default), NMorderColumns is used to reorder the columns before returning the data. NMorderColumns will be called with <code>alpha=FALSE</code> , so columns are not sorted alphabetically. But standard Nonmem columns like ID, TIME, and other will be first. If <code>col.row</code> is used, this will be passed to NMorderColumns too.
<code>check.time</code>	If TRUE (default) and if input data is used, input control stream and input data are checked to be newer than output control stream and output tables. These are important assumptions for the way information is merged by NMscanData. However, if data has been transferred from another system where Nonmem was run, these checks may not make sense, and you may not want to see these warnings. The default can be configured using NMdataConf.

Details

This function makes it very easy to collect the data from a Nonmem run.

A useful feature of this function is that it can automatically combine "input" data (the data read by nonmem in \$INPUT or \$INFILE) with "output" data (tables written by nonmem in \$TABLE). There are two implemented methods for doing so. One (the default but not recommended) relies on interpretation of filter (IGNORE and ACCEPT) statements in \$INPUT. This will work in most cases, and checks for consistency with Nonmem results. However, the recommended method is using a unique row identifier in both input data and at least one output data file (not a FIRSTONLY or LASTONLY table). Supply the name of this column using the `col.row` argument.

Limitations. A number of Nonmem features are not supported. Most of this can be overcome by using `merge.by.row=TRUE`. Incomplete list of known limitations:

- **character TIME**If Nonmem is used to translate DAY and a character TIME column, TIME has to be available in an output table. NMscanData does not do the translation to numeric.
- **RECORDS**The RECORDS option to limit the part of the input data being used is not searched for. Using `merge.by.row=TRUE` will work unaffectedly.
- **NULL**The NULL argument to specify missing value string in input data is not respected. If delimited input data is read (as opposed to rds files), missing values are assumed to be represented by dots (.).

Value

A data set of class 'NMdata'.

See Also

Other DataRead: [NMreadCsv\(\)](#), [NMreadTab\(\)](#), [NMscanInput\(\)](#), [NMscanTables\(\)](#)

Examples

```
res1 <- NMscanData(system.file("examples/nonmem/xgxr001.lst", package="NMdata"))
```

NMscanInput	<i>Find and read input data and optionally translate column names according to the \$INPUT section</i>
-------------	--

Description

Based on a nonmem run (lst and/or mod file), this function finds the input data and reads it. It reads the data like the nonmem run by applying DROP/SKIP arguments and alternative naming of columns in the nonmem run.

Usage

```
NMscanInput(
  file,
  use.rds,
  file.mod,
  dir.data = NULL,
  applyFilters = FALSE,
  translate = TRUE,
  recover.cols = TRUE,
  details = TRUE,
  col.id = "ID",
  col.row,
  quiet,
  args.fread,
  invert = FALSE,
  as.fun
)
```

Arguments

file	a .lst (output) or a .mod (input) control stream file. The filename does not need to end in .lst. It is recommended to use the output control stream because it reflects the model as it was run rather than how it is planned for next run. However, see file.mod and dir.data.
use.rds	If an rds file is found with the exact same name (except for .rds instead of say .csv) as the text file mentioned in the Nonmem control stream, should this be used instead? The default is yes, and NMwriteData will create this by default too.

<code>file.mod</code>	The input control stream file path. Default is to look for <code>"file\"</code> with extension changed to <code>.mod</code> (PSN style). You can also supply the path to the file, or you can provide a function that translates the output file path to the input file path. If <code>dir.data</code> is missing, the input control stream is needed. This is because the <code>.lst</code> does not contain the path to the data file. The <code>.mod</code> file is only used for finding the data file. How to interpret the datafile is read from the <code>.lst</code> file. The default can be configured using <code>NMdataConf</code> . See <code>dir.data</code> too.
<code>dir.data</code>	The data directory can only be read from the control stream (<code>.mod</code>) and not from the output file (<code>.lst</code>). So if you only have the output file, use <code>dir.data</code> to tell in which directory to find the data file. If <code>dir.data</code> is provided, the <code>.mod</code> file is not used at all.
<code>applyFilters</code>	If <code>TRUE</code> (default), <code>IGNORE</code> and <code>ACCEPT</code> statements in the nonmem control streams are applied before returning the data.
<code>translate</code>	If <code>TRUE</code> (default), data columns are named as interpreted by <code>Nonmem</code> (in <code>\$INPUT</code>). If data file contains more columns than mentioned in <code>\$INPUT</code> , these will be named as in data file (if data file contains named variables).
<code>recover.cols</code>	recover columns that were not used in the <code>NONMEM</code> control stream? Default is <code>TRUE</code> . Can only be negative when <code>translate=FALSE</code> .
<code>details</code>	If <code>TRUE</code> , metadata is added to output. In this case, you get a list. Typically, this is mostly useful if programming up functions which behavior must depend on properties of the output. See <code>details</code> .
<code>col.id</code>	The name of the subject ID column. Optional and only used to calculate number of subjects in data. Default is modified by <code>NMdataConf</code> .
<code>col.row</code>	The name of the row counter column. Optional and only used to check whether the row counter is in the data.
<code>quiet</code>	Default is to inform a little, but <code>TRUE</code> is useful for non-interactive stuff.
<code>args.fread</code>	List of arguments passed to <code>fread</code> . Notice that except for <code>"input"</code> and <code>"file"</code> , you need to supply all arguments to <code>fread</code> if you use this argument. Default values can be configured using <code>NMdataConf</code> .
<code>invert</code>	If <code>TRUE</code> , the data rows that are dismissed by the <code>Nonmem</code> data filters (<code>ACCEPT</code> and <code>IGNORE</code>) and only this will be returned. Only used if <code>applyFilters</code> is <code>TRUE</code> .
<code>as.fun</code>	The default is to return data as a <code>data.frame</code> . Pass a function (say <code>tibble::as_tibble</code>) in <code>as.fun</code> to convert to something else. If <code>data.tables</code> are wanted, use <code>as.fun="data.table"</code> . The default can be configured using <code>NMdataConf</code> .

Details

Columns that are dropped (using `DROP` or `SKIP` in `$INPUT`) in the model will be included in the output.

It may not work if a column is dropped, and a new column is renamed to the same name. Say you have `DV` and `CONC` as the only two columns (not possible but illustrative), and in `Nonmem` you do `DV=DROP DV`. Not sure it will work in `Nonmem`, and it probably won't work in `NMscanInput`.

Value

A data set, class defined by `'as.fun'`

See Also

Other DataRead: [NMreadCsv\(\)](#), [NMreadTab\(\)](#), [NMscanData\(\)](#), [NMscanTables\(\)](#)

 NMscanTables

Find and read all output data tables in nonmem run

Description

Find and read all output data tables in nonmem run

Usage

```

NMscanTables(
  file,
  details = FALSE,
  as.fun,
  quiet,
  tab.count = FALSE,
  col.id = "ID",
  col.row
)

```

Arguments

file	the nonmem file to read (normally .mod or .lst)
details	If TRUE, metadata is added to output. In this case, you get a list. Typically, this is mostly useful if programming up functions which behavior must depend on properties of the output.
as.fun	The default is to return data as a data.frame. Pass a function (say <code>tibble::as_tibble</code>) in <code>as.fun</code> to convert to something else. If data.tables are wanted, use <code>as.fun="data.table"</code> . The default can be configured using <code>NMdataConf</code> .
quiet	The default is to give some information along the way on what data is found. But consider setting this to TRUE for non-interactive use. Default can be configured using <code>NMdataConf</code> .
tab.count	Nonmem includes a counter of tables in the written data files. These are often not useful. However, if <code>tab.count</code> is TRUE (not default), this will be carried forward and added as a column called <code>TABLENO</code> .
col.id	name of the subject ID column. Used for calculation of the number of subjects in each table.
col.row	The name of the row counter column. Optional and only used to check whether the row counter is in the data.

Value

A list of all the tables as data.frames. If `details=TRUE`, this is in one element, called `data`, and `meta` is another element. If not, only the data is returned.

See Also

Other DataRead: [NMreadCsv\(\)](#), [NMreadTab\(\)](#), [NMscanData\(\)](#), [NMscanInput\(\)](#)

Examples

```
tabs1 <- NMscanTables(system.file("examples/nonmem/xgxr001.lst", package="NMdata"))
```

NMstamp	<i>stamp a dataset or any other object</i>
---------	--

Description

Dataset metadata can be valuable, eg. by tracing an archived dataset back to the code that generated it. The metadata added by NMstamp can be accessed using the function NMinfo.

Usage

```
NMstamp(data, script, time = Sys.time(), ...)
```

Arguments

data	The dataset to stamp.
script	path to the script where the dataset was generated.
time	the time stamp to attach. Default is to use cpu clock.
...	other named metadata elements to add to the dataset. Example: Description="PK data for ph1 trials in project".

Details

NMstamp modifies the meta data by reference. See example.

Value

data with meta data attached. Class unchanged.

See Also

NMinfo

Other DataCreate: [NMorderColumns\(\)](#), [findCovs\(\)](#), [findVars\(\)](#), [flagsAssign\(\)](#), [flagsCount\(\)](#), [mergeCheck\(\)](#), [tmpcol\(\)](#)

Examples

```
x=1
NMstamp(x,script="example.R",description="Example data")
NMinfo(x)
```

 NMwriteData

Write dataset for use in Nonmem (and R)

Description

Instead of trying to remember the arguments to pass to write.csv, use this wrapper. It tells you what to write in \$DATA and \$INPUT in nonmem, and it (additionally) exports an rds or Rdata file as well which is highly preferable for use in R. It never edits the data before writing the datafile. The filenames for csv, rds etc. are derived by replacing the extension to the filename given in the file argument.

Usage

```

NMwriteData(
  data,
  file,
  write.csv = TRUE,
  write.rds = write.csv,
  write.RData = FALSE,
  script,
  args.stamp,
  args.fwrite,
  args.rds,
  args.RData,
  quiet,
  args.NMgenText,
  nm.drop,
  nmdir.data,
  col.flagn,
  nm.rename,
  nm.copy,
  nm.capitalize,
  allow.char.TIME
)

```

Arguments

data	The dataset to write to file for use in Nonmem.
file	The file to write to. The extension (everything after and including last ".") is dropped. csv, rds and other standard file name extensions are added.
write.csv	Write to csv file?
write.rds	write an rds file?
write.RData	In case you want to save to .RData object. Not recommended. Use write.rds instead.
script	If provided, the object will be stamped with this script name before saved to rds or Rdata. See ?NMstamp.

<code>args.stamp</code>	A list of arguments to be passed to NMstamp.
<code>args.fwrite</code>	List of arguments passed to fwrite. Notice that except for "x" and "file", you need to supply all arguments to fwrite if you use this argument. Default values can be configured using NMdataConf.
<code>args.rds</code>	A list of arguments to be passed to saveRDS.
<code>args.RData</code>	A list of arguments to be passed to save.
<code>quiet</code>	The default is to give some information along the way on what data is found. But consider setting this to TRUE for non-interactive use. Default can be configured using NMdataConf.
<code>args.NMgenText</code>	List of arguments to pass to NMgenText - the function that generates text suggestion for INPUT and DATA sections in the NONMEM control stream. You can use these arguments to get a text suggestion you can use directly in NONMEM - and NwriteSection can even update multiple NONMEM control streams based on the result. This will update your control streams to match your new data file with just one command.
<code>nm.drop</code>	Deprecated, use <code>args.NMgenText=list(drop=c("column"))</code> instead.
<code>nmdir.data</code>	Deprecated, use <code>args.NMgenText=list(dir.data="your/path")</code> instead.
<code>col.flagn</code>	Name of a numeric column with zero value for rows to include in Nonmem run, non-zero for rows to skip. The argument is only used for generating the proposed \$DATA text to paste into the Nonmem control stream. To skip this feature, use <code>col.flagn=NULL</code> .
<code>nm.rename</code>	Deprecated, use <code>args.NMgenText=list(rename=c(newname="existing"))</code> instead.
<code>nm.copy</code>	Deprecated, use <code>args.NMgenText=list(copy=c(newname="existing"))</code> instead.
<code>nm.capitalize</code>	Deprecated, use <code>args.NMgenText=list(capitalize=TRUE)</code> instead.
<code>allow.char.TIME</code>	Deprecated, use <code>args.NMgenText=list(allow.char.TIME=TRUE)</code> instead.

Details

When writing csv files, the file will be comma-separated. Because Nonmem does not support quoted fields, you must avoid commas in character fields. An error is returned if commas are found in strings.

The user is provided with text to use in Nonmem. This lists names of the data columns. Once a column is reached that Nonmem will not be able to read as a numeric and column is not in `nm.drop`, the list is stopped. Only exception is `TIME` which is not tested for whether character or not.

Value

Text for inclusion in Nonmem control stream, invisibly.

See Also

Other Nonmem: [NMapplyFilters\(\)](#), [NMextractText\(\)](#), [NMgenText\(\)](#), [NMreadSection\(\)](#), [NMwriteSection\(\)](#)

NMwriteSection	<i>Replace (\$)sections of a nonmem control stream</i>
----------------	--

Description

Just give the section name, the new lines and the file path, and the "\$section", and the input to Nonmem will be updated.

Usage

```
NMwriteSection(
  files,
  file.pattern,
  dir,
  section,
  newlines,
  list.sections,
  newfile,
  backup = TRUE,
  blank.append = TRUE,
  data.file,
  write = TRUE,
  quiet,
  simplify = TRUE
)
```

Arguments

files	File paths to the models (control stream) to edit. See file.pattern too.
file.pattern	Alternatively to files, you can supply a regular expression which will be passed to list.files as the pattern argument. If this is used, use dir argument as well. Also see data.file to only process models that use a specific data file.
dir	If file.pattern is used, dir is the directory to search in.
section	The name of the section to update without "\$". Example: section="EST" to edit the sections starting by \$EST. Section specification is not case-sensitive. See ?NMreadSection too.
newlines	The new text (including "\$SECTION"). Better be broken into lines in a character vector since this is simply past to writeLines.
list.sections	Named list of new sections, each element containing a section. Names must be section names, contents of each element are the new section lines for each section.
newfile	path to new run. If missing, path is used. If NULL, output is returned rather than written.
backup	In case you are overwriting the old file, do you want to backup the file (to say, backup_run001.mod)?

blank.append	Append a blank line to output?
data.file	Use this to limit the scope of models to those that use a specific input data data file. The string has to exactly match the one in \$DATA or \$INFILE in Nonmem.
write	Default is to write to file. If write=FALSE, NMwriteSection returns the resulting input.txt without writing it. to disk? Default is FALSE.
quiet	The default is to give some information along the way on what data is found. But consider setting this to TRUE for non-interactive use. Default can be configured using NMdataConf.
simplify	If TRUE (default) and only one file is edited, the resulting rows are returned directly. If more than one file is edited, the result will always be a list with one element per file.

Details

The new file will be written with unix-style line endings.

Value

The new section text is returned. If write=TRUE, this is done invisibly.

See Also

Other Nonmem: [NMapplyFilters\(\)](#), [NMextractText\(\)](#), [NMgenText\(\)](#), [NMreadSection\(\)](#), [NMwriteData\(\)](#)

Examples

```
newlines <- "$EST POSTHOC INTERACTION METHOD=1 NOABORT PRINT=5 MAXEVAL=9999 SIG=3"
NMwriteSection(files=system.file("examples/nonmem/xgxr001.mod", package = "NMdata"),
section="EST", newlines=newlines,newfile=NULL)
```

print.summary_NMdata *print method for NMdata summaries*

Description

print method for NMdata summaries

Usage

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

Arguments

x The summary object to be printed. See ?summary.NMdata
... Arguments passed to other print methods.

renameByContents	<i>Rename columns matching properties of data contents</i>
------------------	--

Description

For instance, lowercase all columns that Nonmem cannot interpret (as numeric).

Usage

```
renameByContents(data, fun.test, fun.rename, invert.test = FALSE, as.fun)
```

Arguments

data	data.frame in which to rename columns
fun.test	Function that returns TRUE for columns to be renamed.
fun.rename	Function that takes the existing column name and returns the new one.
invert.test	Rename those where FALSE is returned from fun.test.
as.fun	The default is to return data as a data.frame. Pass a function (say <code>tibble::as_tibble</code>) in <code>as.fun</code> to convert to something else. If data.tables are wanted, use <code>as.fun="data.table"</code> . The default can be configured using <code>NMdataConf</code> .

Value

data with (some) new column names. Class as defined by `as.fun`.

Examples

```
pk <- readRDS(file=system.file("examples/data/xgxr2.rds", package="NMdata"))
pk[,trtact:=NULL]
pk <- renameByContents(data=pk,
                       fun.test = NMisNumeric,
                       fun.rename = tolower,
                       invert.test = TRUE)
## Or append a "C" to the same column names
pk <- readRDS(file=system.file("examples/data/xgxr2.rds", package="NMdata"))
pk[,trtact:=NULL]
pk <- renameByContents(data=pk,
                       fun.test = NMisNumeric,
                       fun.rename = function(x)paste0(x, "C"),
                       invert.test = TRUE)
```

summary.NMdata	<i>summary method for NMdata objects</i>
----------------	--

Description

summary method for NMdata objects

Usage

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

Arguments

object	An NMdata object (from NMscanData).
...	Only passed to the summary generic if object is missing NMdata meta data (this should not happen anyway).

Details

The subjects are counted conditioned on the nmout column. If only id-level output tables are present, there are no nmout=TRUE rows. This means that in this case it will report that no IDs are found in output. The correct statement is that records are found for zero subjects in output tables.

Value

A list with summary information on the NMdata object.

unNMdata	<i>Remove NMdata class and discard NMdata meta data</i>
----------	---

Description

Remove NMdata class and discard NMdata meta data

Usage

```
unNMdata(x)
```

Arguments

x	An 'NMdata' object.
---	---------------------

Value

x stripped from the 'NMdata' class

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