Package ‘NMproject’

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Type Package

Title Script Based 'NONMEM' Model Development

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BugReports https://github.com/tsahota/NMproject/issues

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Description Industrialisation of 'NONMEM' <https://www.iconplc.com/innovation/nonmem/> via fully and rapidly reusable model development 'workflows' entirely within 'RStudio'. Quickly get started with new models by importing 'NONMEM' templates from the built-in code library. Manipulate 'NONMEM' code from within R either via the tracked 'manual edit' interface or 'programmatically' via convenience functions. Script 'workflows' by piping sequences of model building steps from control file creation, to execution, to post-processing and evaluation. Run caching makes 'workflows' R markdown friendly for easy documentation of thoughts and modelling decisions alongside executable code. Share, reuse and recycle 'workflows' for new problems.

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Encoding UTF-8

Imports shiny, reshape2, dygraphs, DT, git2r (>= 0.18.0), dplyr (>= 0.7.2), methods, stringr (>= 1.3.1), rlang (>= 0.2.1), diffobj (>= 0.1.11), tidyr, miniUI (>= 0.1.1), rstudioapi (>= 0.7), crayon (>= 1.3.4), rprojroot, htmltools, rmarkdown, magrittr, usethis, lifecycle (>= 1.0.0)

RoxygenNote 7.1.1

Suggests testthat, knitr, ggplot2, future, data.tree, xpose, lubridate, pmxTools, Hmisc, rsample, renv, desc, purrr, digest, covr, devtools, roxygen2

Collate 'NMproject-options.R' 'NMproject-package.R' 'Vectorize.R' 'addin-apps.R' 'apply_manual_edit.R' 'basic-ctl-manipulation.R'
\texttt{R topics documented:}

```
'utils.R' 'basic_methods.R' 'boot.R' 'nm_object.R' 'cache.R'
'covariate-explore.R' 'cran_note_handle.R' 'data_filter.R'
'decision.R' 'deprecated.R' 'derived-data-prep.R'
'developer-funs.R' 'directory-management.R' 'dollar_input.R'
'find-nomem.R' 'import-code.R' 'init_funs.R' 'input_data.R'
'job_stats.R' 'low-level-ctl-handling-funs.R'
'make_OCC_every_dose.R' 'make_project.R' 'manual-edit.R'
'monitoring.R' 'nm-gettersetters.R' 'nm_diff.R'
'nm_read_table.R' 'nm_render.R' 'nm_tran.R' 'nm_tree.R'
'nmsave.R' 'ofv.R' 'output_table.R' 'param-manipulate.R'
'plot_iter.R' 'post-run-summaries.R' 'prompt_overwrite.R'
'psn_style_scm.R' 'read_ext.R' 'rmd_to_vignette.R' 'run_nm.R'
'shiny-apps.R' 'show-file.R' 'sim-diagnostics.R'
'snippet_setup.R' 'stepwise-covariate.R' 'subroutine.R'
'system-hooks.R' 'text.R' 'update_parameters.R'
'with_temp_git_config.R' 'zzz.R'
```

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add_mixed_param

Add a mixed effect parameter to $PK$ (or $PRED$)

Description

[Stable]

Primarily an internal function. This will (by default) add a parameter (mixed effect) to your code $PK/PRED$ and $\Theta/\Omega$. 
### Usage

```r
add_mixed_param(
  m,
  name,
  init = 1,
  unit = "",
  trans = c("LOG"),
  position = NA_integer_,
  after = character()
)
```

### Arguments

- `m`: An nm object.
- `name`: Character. Name of NONMEM variable to create.
- `init`: Numeric (default = 1). Initial value of fixed effect.
- `unit`: Character (default = ""). Unit of variable.
- `trans`: Character (default = "LOG"). Transformation of the variable.
- `position`: Integer. Not used.
- `after`: Character. Pattern to match and include the mixed effect after.

### Value

An nm object with modified ctl_contents field.

### Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("PK")
m1 %>% dollar("THETA")

m1 <- m1 %>% add_mixed_param("ALAG1", init = 1.1, unit = "h", trans = "LOG")

m1 %>% dollar("PK")
m1 %>% dollar("THETA")
```
add_remove_covs  
Add/remove a covariate to a NONMEM model

Description

[Stable]
Follows PsN coding conventions to add covariates into a model. The advantage is no need to create a .scm file, just directly modify the NONMEM control file contents. This function is used by `covariate_step_tibble()` for stepwise covariate model development.

Usage

```r
add_cov(
  ctl,  
  param,  
  cov,  
  state = 2,  
  continuous = TRUE,  
  time_varying,  
  additional_state_text = list(),  
  id_var = "ID",  
  force = FALSE,  
  force_TV_var = FALSE,  
  init,  
  lower,  
  upper
)
```

```r
remove_cov(
  ctl,  
  param,  
  cov,  
  state = 2,  
  continuous = TRUE,  
  time_varying,  
  id_var = "ID"
)
```

Arguments

- `ctl`  
  An nm object or an object coercible to `ctl_list`.  
- `param`  
  Character. Name of parameter.  
- `cov`  
  Character. Name of covariate.  
- `state`  
  Numeric or character. Number or name of state (see details).  
- `continuous`  
  Logical (default = TRUE). Is covariate continuous?
time_varying  Optional logical. is the covariate time varying?
additional_state_text Optional character (default = empty). Custom state variable to be passed to param_cov_text.
id_var Character (default = "ID"). Needed if time_varying is missing.
force Logical (default = 'FALSE'). Force covariate in even if missing values found.
force_TV_var Logical (default = FALSE). Force covariates only on TV notation parameters.
init Optional numeric/character vector. Initial estimate of additional parameters.
lower Optional numeric/character vector. lower bound of additional parameters.
upper Optional numeric/character vector. Upper bound of additional parameters.

Details

Available states:

"2" or "linear"  PARCOV= (1 + THETA(1)*(COV - median))
"3" or "hockey-stick"  IF(COV.LE.median) PARCOV = (1 + THETA(1)*(COV - median)) IF(COV.GT.median)
                     PARCOV = (1 + THETA(2)*(COV - median))
"4" or "exponential"  PARCOV = EXP(THETA(1)*(COV - median))
"5" or "power"  PARCOV = ((COV/median)**THETA(1))
"power1"  PARCOV = ((COV/median))
"power0.75"  PARCOV = ((COV/median)**0.75)
"6" or "log-linear"  PARCOV = (1 + THETA(1)*(LOG(COV) - log(median)))

remove_cov only works with covariates added with add_cov.

Value

An nm object with modified ctl_contents field.

See Also

covariate_step_tibble(), test_relations()

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

## dataset has missing WT so create a new one and assign this to the run
input_data(m1) %>%

```r
dplyr::group_by(ID) %>%
dplyr::mutate(WT = na.omit(WT)) %>%
write_derived_data(temp_data_file)

m1 <- m1 %>% data_path(temp_data_file)

m1WT <- m1 %>% child("m1WT") %>%
  add_cov(param = "V", cov = "WT", state = "power")

m1 %>% dollar("PK")

m1WT %>% dollar("PK") # notice SCM style code added

nm_diff(m1WT)

# Not run:
run_nm(c(m1, m1WT))
rr(c(m1, m1WT))
summary_wide(c(m1, m1WT))

# End(Not run)
unlink(temp_data_file)

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

temp_data_file <- paste0(tempfile(), ".csv")

# dataset has missing WTs so create a new one and assign this to the run
input_data(m1) %>%
dplyr::group_by(ID) %>%
dplyr::mutate(WT = na.omit(WT)) %>%
write_derived_data(temp_data_file)

m1 <- m1 %>% data_path(temp_data_file)

m1WT <- m1 %>% child("m1WT") %>%
  add_cov(param = "V", cov = "WT", state = "power")

m1 %>% dollar("PK")

m1WT %>% dollar("PK") # notice SCM style code added

# reverse this by removing WT
m1noWT <- m1WT %>% child("m1noWT") %>%
  remove_cov(param = "V", cov = "WT")

m1noWT %>% dollar("PK")

m1noWT %>% dollar("THETA")
```
append_nonmem_var

unlink(temp_data_file)

append_nonmem_var  Include NONMEM variables in output table

Description

[Experimental]
This is designed to be used in situations where you don’t want to rerun NONMEM, but need a variable defined in the control file. This will parse the $PK/$PRED" and compute it as an additional row in R. Safest way is to just rerun the model with the variable in $TABLE, but this is for those who are too time constrained. It is advisable to QC the output.

Usage

append_nonmem_var(output_table, r, var)

Arguments

output_table  Output from output_table().
r  An nm object.
var  Character. Name of variable to extract (needs to be defined in $PK/$PRED).

Value

A modified version of output_table with addition var column.

apply_manual_edit  Apply a manual edit patch

Description

[Stable]
It is best to allow the "manual edit" RStudio ‘Addin’ to write this function in your script for you. After a tracked manual edit is performed, a patch file is created and saved in the "patches" subdirectory of nm_dir("models"). This function applies the patch to the object.

Usage

apply_manual_edit(m, patch_id, return_merge_conf_ctl = FALSE)
bind_covariate_results

Arguments

- m: An nm object.
- patch_id: Character name of patch. Corresponds to the file name in the "patches" subdirectory of nm_dir("models").
- return_merge_conf_ctl: Logical (default = FALSE). If there a merge conflict produced, should the ctl file be returned?

Details

Generally best to to apply patches before automatic edits and changes in directories e.g. via run_in(). If patches are applied to NONMEM control file sections that are likely to change in the future, the patch may fail to apply. In this case, it is best to view the patch (via the "view patch" RStudio 'Addin') and manually re-implement the changes again in a new manual edit.

Value

An nm object with modified ctl_contents field.

bind_covariate_results

Add run results into a covariate tibble

Description

[Stable]

Extracts results from completed covariate runs and combines them into the covariate tibble().

The goal of NMproject’s covariate modelling functions is to provide a stepwise covariate method with manual decision making. This important to ensure that the full model selection/evaluation criteria (should be defined in statistical analysis plans) can be applied at every step rather than just log likelihood ratio testing, where the most significant model may be unstable, may worsen model predictions or may only be slightly more significant than a more physiologically plausible covariate relationship.

The functions test_relations(), covariate_step_tibble(), bind_covariate_results() together comprise NMproject stepwise covariate method with manual decision. The goal is to be part way between PsN’s SCM and completely manual process at each forward and backward elimination step. The syntax of how covariates are included is the same as PsN’s SCM routine - See PsN documentation for more information.

Usage

bind_covariate_results(dsc, nm_col = "m", parameters = "new")
Arguments

- **dsc**  
  An output tibble from `covariate_step_tibble()`.

- **nm_col**  
  Character (default = "m"). Name of column to store nm objects.

- **parameters**  
  Character (default = "new"). Passed to `summary_wide()`.

Value

An modified version of `dsc` with additional columns from `summary_wide()` for model selection purposes.

See Also

- `covariate_step_tibble()` and `nm_render()` for rendering diagnostic reports for (subsets of) models in `nm_col`.

Examples

```r
## requires NONMEM to be installed
## Not run:
## create tibble of covariate step with model objects as column m
dsm1 <- m1 %>% covariate_step_tibble(
  run_id = "m1_f1",
  dtest = dtest,
  direction = "forward"
)

## run all models greedily
dsm1$m <- dsm1$m %>% run_nm()

wait_finish(dsm1$m)

## extract results and put into tibble
dsm1 <- dsm1 %>% bind_covariate_results()

## plot goodness of fit diagnostics top 3 models (in terms of p-value)
dsm1$m[1:3] %>% nm_render("Scripts/basic_gof.Rmd")
```

## End(Not run)

---

**block-omega-sigma**  
Create or remove $OMEGA/$SIGMA BLOCKs

---

**Description**

[Stable]

Manipulate $OMEGA$ (and $SIGMA$) BLOCKs to introduce or remove correlations.
Usage

`block(iomega, eta_numbers = NA, diag_init = 0.01)`

`unblock(iomega, eta_numbers)`

Arguments

- `iomega` A tibble output from `init_omega()` or `init_sigma()`.
- `eta_numbers` Numeric vector. ETA numbers to put into a block or unblock for `block()` and `unblock()`, respectively. Must be contiguous.
- `diag_init` Numeric. Default value for off diagonal elements.

Value

An nm object with modified ctl_contents field.

See Also

`init_theta()`, `init_omega()`, `init_sigma()`

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

io <- m1 %>% init_omega()
io <- io %>% block(c(2, 3))
m1 <- m1 %>% init_omega(io)
m1 %>% dollar("OMEGA") ## to display $OMEGA

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

## first create a block
io <- m1 %>% init_omega()
io <- io %>% block(c(2, 3))
m1 <- m1 %>% init_omega(io)
m1 %>% dollar("OMEGA") ## to display $OMEGA

## now unblock
io <- io %>% unblock(c(2, 3))
m1 <- m1 %>% init_omega(io)
```
child

m1 %>% dollar("OMEGA") ## to display $OMEGA

##

---

**child**

*Make child nm object from parent*

### Description

[Stable]

Child objects inherit attributes of parent but with a new `run_id`. The control file will be inherited too with $TABLEs updated.

### Usage

```r
child(m, run_id = NA_character_, type = "execute", parent = m, silent = FALSE)
```

### Arguments

- **m**
  - Parent nm object.
- **run_id**
  - Character. New `run_id` to assign to child object.
- **type**
  - Character (default = "execute"). Type of child object.
- **parent**
  - Optional nm object (default = `m`). Parent object will by default be `m`, but this argument will force parent to be a different object.
- **silent**
  - Logical (default = FALSE). Should warn if conflicts detected.

### Details

Specifying `parent` will force parent to be different from `m`. This is useful in piping when a parent object is modified prior to being used in the child object.

### Value

An new nm object with modified parent_\* fields updated to be the \* fields of the parent object, `m`.

### Examples

```r
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m2 <- m1 %>% child("m2")

nm_diff(m2, m1)
```
**code_library**  

**Description**  

Function not designed for direct use. Instead use the RStudio code library entry on the RStudio 'Addins' menu. This will open the shiny app. Select the file, and click "preview" to view and `import()` to bring into the "staging" area of your project. See vignette at [https://tsahota.github.io/NMproject/](https://tsahota.github.io/NMproject/) for a video showing use of the app. NONMEM control files will intentionally not be imported straight in the "Models" directory and instead go into "staging/Models". This staging location can be referred to when creating `nm` objects with `new_nm(..., based_on = "staging/Models/[filename]")`.

**Usage**  

```r  
code_library(  
extn = NULL,  
fields = "Description",  
viewer = TRUE,  
silent = FALSE,  
return_info = FALSE  
)  
```

**Arguments**  

- `extn`: Vector string of extensions to include (default = NULL includes all).
- `fields`: Character vector of fields to extract.
- `viewer`: Logical indicating if viewer should be used to display results (default=FALSE).
- `silent`: Logical indicating if messages should be silenced (default=FALSE).
- `return_info`: Logical (default = FALSE). Return data.frame of results (FALSE= returns file paths).

**Details**  

Requires `getOption("code_library_path")` to be set.

**Value**  

If `return_info = TRUE`, invisibly returns output a tibble with code library information. Otherwise (this may be deprecated soon), will return paths to code library files.

**See Also**  

`ls_code_library(), stage(), import()`
Examples

code_library(viewer = FALSE, return_info = TRUE)

coef_widelong  Extract parameter values

Description

[Stable]
Pulls parameters, standard errors, OFVs and condition numbers out of ext files, applies transformations. This function is useful when numeric values are needed. \texttt{rr} is easier to read, however it returns characters. A wide and long format is available via two different functions.

Usage

c coef_wide(m, trans = TRUE)

c coef_long(m, trans = TRUE)

Arguments

m An \texttt{nm} object.
trans Logical (default = \texttt{TRUE}). Transform parameters using comments in $\text{T}\text{HET}\text{A}$/\$\text{OM}\text{E}\text{G}\text{A}/\$\text{S}\text{I}\text{G}\text{MA}.

Value

data.frame of extracted model parameter values. \texttt{coef_wide()} returns a data.frame in wide format. Vector valued objects \texttt{m}, will be stacked vertically with one row per run. \texttt{coef_long()} returns a data.frame in long format. Vector valued objects \texttt{m}, will be stacked horizontally.

NONMEM coding conventions used by NMproject

The convention for $\text{T}\text{HET}\text{A}$ comments used by NMproject is value ; name ; unit ; transformation

e.g. $\text{T}\text{HET}\text{A} 0.1 ; \text{KA} ; h^{-1} ; \text{LOG}$

The options for \text{T}\text{HET}\text{A} transformations are: \texttt{LOG}, \texttt{LOGIT}, \texttt{RATIO} and missing. \texttt{LOG} and \texttt{LOGIT} refer to log and logit transformed \text{T}\text{HET}\text{A}s, respectively where the parameters should be back-transformed for reporting. \texttt{RATIO} refers to ratio data types, i.e. parameters that are positive and have a meaningful zero. Most parameters like KA, CL, EMAX fall into this category, but covariates effects which can go negative do not. RSEs are calculated for ratio data. Missing transformations are suitable for all other parameters, here no RSEs will be calculated, only raw SE values will be reported.

The convention for $\text{OM}\text{E}\text{G}\text{A}$ is similar but without a unit item: value ; name ; transformation

e.g. $\text{OM}\text{E}\text{G}\text{A} 0.1 ; \text{IIV\_KA} ; \text{LOG}$
The options for OMEGA are either LOG or missing. LOG indicating that the individual parameter distribution is log normally distributions and should be reported as a CV% (and associated RSE%) rather than as the raw NONMEM estimate.

The convention for $OMEGA is just : value ; name.

**THETA transformations using trans = TRUE**

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\theta$ and $se(\theta)$ are the NONMEM reported values of parameters and standard errors, respectively:

1. **LOG** $FINAL = exp(\theta), RSE = 100\sqrt{exp(se(\theta)^2) - 1}$
2. **RATIO** $FINAL = \theta, RSE = 100se(\theta)/\theta$
3. **LOGIT** $FINAL = 100/(1 + exp(-\theta)), SE = se(\theta)$
4. **missing** $FINAL = \theta, SE = se(\theta)$

**OMEGA transformations using trans = TRUE**

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\omega^2$ and $se(\omega^2)$ are the NONMEM reported values of parameters and standard errors, respectively:

1. **LOG** $FINAL = 100\sqrt{exp(\omega^2) - 1}, RSE = 100(se(\omega^2)/\omega^2)/2$
2. **missing** $FINAL = \omega^2, SE = se(\omega^2)$

**SIGMA transformations using trans = TRUE**

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\sigma^2$ and $se(\sigma^2)$ are the NONMEM reported values of parameters and standard errors, respectively. All sigmas are reported as standard deviations.

1. **all sigmas** $FINAL = \sqrt(\sigma^2), RSE = 100se(\sigma^2)/\sigma^2$

See Also

rr()
comment_lines  
Comment and uncomment lines of control file

**Description**  
[Stable]  
Comment out lines of code with that are matched by a patter string.

**Usage**  

```r
comment_out(m, pattern = ".*")
uncomment(m, pattern = ".*")
```

**Arguments**  

- `m`  
  An nm object.

- `pattern`  
  Character regex. Passed to `gsub()`.

**Value**  
An nm object with modified `ctl_contents` field.

**See Also**  

- `gsub_ctl()`, `target()`  

---

cond_num  
Condition number of run

**Description**  
[Stable]  
Extracts condition number from .ext file.

**Usage**  

```r
cond_num(r)
```

**Arguments**  

- `r`  
  An nm object.

**Value**  
The numeric value of the condition number.
convert_to_simulation

See Also

ofv(), rr()

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

is_finished(m1) ## FALSE until run is completed
cond_num(m1) ## NA until m1 is finished

convert_to_simulation  Convert a NONMEM run to a simulation

Description

[Stable]

Replaces $EST with $SIM.

Usage

convert_to_simulation(m, seed = 12345, subpr = 1)

Arguments

m           A nm object.
seed        Numeric (default = 12345). seed value to include in $SIM.
subpr       Numeric (default = 1). SUBPR value to include in $SIM.

Details

Will only change $EST/$SIM, therefore it will not be sufficient to change a categorical estimation control file to simulation. You will likely need to perform a manual edit for categorical data simulation.

Value

An nm object with modified ctl_contents field.
covariance_plot

Examples

```r
## Not run:
## requires NONMEM to be installed
m1s <- m1 %>%
  child(run_id = "m1s") %>%
  update_parameters(m1) %>%
  convert_to_simulation(subpr = 50) %>%
  run_nm()

m1s %>% nm_render("Scripts/basic_vpc.Rmd")
m1s %>% nm_render("Scripts/basic_ppc.Rmd")

## End(Not run)
```

covariance_plot  Plot $COV$ matrix

Description

[Stable]

Usage

covariance_plot(r, trans = TRUE)

Arguments

- `r` An nm object.
- `trans` Logical (default = TRUE). Applies the transformations specified in $THETA$/SOMEGA/$SIGMA$ comments before plotting.

Details

Plots the correlation plot from the $COV$ NONMEM output.

Value

A ggplot2 object with parameter correlations.

See Also

- `nm_render()`
covariate_step_tibble

Prepare forward covariate step

Description

[Stable]

Takes a base nm object and a set of relationships to test (from test_relations()) and prepares a tibble of NONMEM runs.

The goal of NMproject’s covariate modelling functions is to provide a stepwise covariate method with manual decision making. This important to ensure that the full model selection/evaluation criteria (should be defined in statistical analysis plans) can be applied at every step rather than just log likelihood ratio testing, where the most significant model may be unstable, may worsen model predictions or may only be slightly more significant than a more physiologically plausible covariate relationship.

The functions test_relations(), covariate_step_tibble(), bind_covariate_results() together comprise NMproject stepwise covariate method with manual decision. The goal is to be part way between PsN’s SCM and completely manual process at each forward and backward elimination step. The syntax of how covariates are included is the same as PsN’s SCM routine - See PsN documentation for more information.

Usage

```r
covariate_step_tibble(
  base,
  run_id,
  run_in = nm_dir("models"),
  dtest,
  direction = c("forward", "backward"),
  ...
)
```

Arguments

- **base**: An nm object.
- **run_id**: Base run_id to construct run_ids of covariate runs.
covariate_step_tibble

run_in Character. See `run_in()`.

dtest dplyr::tibble with testing relations (from `test_relations()`).

direction Character. "forward" (default) or "backward".

... Additional arguments passed to `add_cov()`.

Value

Will return dtest a dplyr::tibble with appended columns.

See Also

test_relations(), bind_covariate_results(), add_cov()

Examples

dtest <- test_relations(param = c("KA", "K", "V"),
                      cov = c("LIN1", "LIN2", "LIN3", "RND1", "RND2", "RND3"),
                      state = c("linear", "power"),
                      continuous = TRUE) %>%
test_relations(param = c("KA", "K", "V"),
               cov = "BN1",
               state = "linear",
               continuous = FALSE)

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

temp_data_file <- paste0(tempfile(), ".csv")

## dataset has missing WTs so create a new one and assign this to the run
input_data(m1) %>%
dplyr::group_by(ID) %>%
dplyr::mutate(WT = na.omit(WT)) %>%
write_derived_data(temp_data_file)

m1 <- m1 %>% data_path(temp_data_file)

# test_relations

dtest <- test_relations(param = c("K", "V"),
                       cov = c("WT"),
                       state = c("linear", "power"),
                       continuous = TRUE)

# requires NONMEM to be installed
## Not run:
## create tibble of covariate step with model objects as column m
dsm1 <- m1 %>% covariate_step_tibble(run_id = "m1_f1",
                                     dtest = dtest,
## run all models greedily
```
dsm1$m <- dsm1$m %>% run_nm()
```

## extract results and put into tibble
```
dsm1 <- dsm1 %>% bind_covariate_results()
```

## sort by BIC (for example) and view
```
dsm1 <- dsm1 %>% arrange(BIC)
dsm1
```

## check condition number, covariance,...
## run any diagnostics here

## when happy with selection, select run for subsequent step
```
m1_f1 <- dsm1$m[1]  ## select most significant BIC
```

# alternative select by relationship
```
m1_f1 <- dsm1 %>%
  filter(param = "CL", cov = "BWT", state = "power") %>%
m
```

## do next forward step
```
dsm2 <- m1_f1 %>% covariate_step_tibble(run_id = "m1_f2",
                                     dtest = dtest,
                                     direction = "forward")
```

## continue ...

## End(Not run)

---

**cov_cov_plot**

*Plot correlation between two covariates*

**Description**

[Stable]
Useful for exploratory plots.

**Usage**

```
cov_cov_plot(
  d,  
cov,  
continuous,  
log_transform_plot = rep(FALSE, length(cov)),  
dcov_info,  
by = "ID"
)
```
cov_forest_data

Arguments

d  Dataset with covariates.
cov  Vector of length 2 for covariate names.
continuous  Logical vector of length 2 for whether cov is continuous or not.
log_transform_plot  Should plot be log transformed or not.
dcov_info  Optional data.frame with covariate information.
by  Character (default = "ID") variable to split over.

Value

ggplot2 object displaying covariate-covariate correlations.

Description

[Stable]

The main workhorse for computing uncertainty quantiles of covariate effects in different subpopulations.

Usage

cov_forest_data(m, covariate_scenarios)

Arguments

m  An mm object.
covariate_scenarios  A data.frame. Need columns cov, value and (optional) text. See details for more information.

Details

The column cov in covariate_scenarios refers to covariate variables in the dataset. The column value refers to covariate values of importance. Typically these will be quantiles of continuous variables and categories (for categorical covariates). The column text is option but is a labelling column for cov_forest_plot() to adjust how the covariate scenarios are printed on the axis.

Value

dplyr::tibble with quantile information suitable for cov_forest_plot().
## cov_forest_data

**Description**

[Stable]

Uses ggplot2 to take outputs from `cov_forest_data()` and display a forest plot.

**Usage**

```r
cov_forest_plot(d)
```

**Arguments**

- `d` 
  
  A data frame from `cov_forest_data()`.

**Value**

A ggplot2 forest plot.

**See Also**

`cov_forest_data()`
Examples

```r
## requires NONMEM to be installed
## Not run:

dcov <- input_data(m1, filter = TRUE)
dcov <- dcov[!duplicated(dcov$ID), ]
covariate_scenarios <- bind_rows(
  tibble(cov = "HEALTHGP", value = c(0, 1)),
  tibble(cov = "HEPATIC", value = unique(dcov$HEPATIC[, dcov$HEPATIC > -99])),
  tibble(cov = "BWTIMP", value = c(50, 80, 120)),
  tibble(cov = "ECOG", value = c(0, 1, 2, 3)),
  tibble(cov = "BEGFRIMP", value = quantile(dcov$BEGFR[, dcov$BEGFR > -99])),
  tibble(cov = "RACE", value = c(1, 2), text = c("white", "black")),
  tibble(cov = "PPI", value = c(0, 1)),
  tibble(cov = "HZRA", value = c(0, 1))
)

dplot <- cov_forest_data(m1, covariate_scenarios = covariate_scenarios)
cov_forest_plot(dplot)

## End(Not run)
```

### ctl_contents

**Get/set control file contents**

#### Description

This function is an alias for `based_on()`.

#### Usage

```r
ctl_contents(...)
```

#### Arguments

... 

Arguments to be passed to `based_on()`.

#### Value

An nm object with modified `ctl_contents` field.

#### Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1")
```
Get and set path to NONMEM control file

Description

[Stable]
Similar to `ctl_name()` & `run_in()`, this allows you to retrieve and specify the relative path to the control file that will be written by the `run_nm()`.

Usage

```r
ctl_path(m, text)
```

Arguments

- `m` An `nm` object.
- `text` Optional character. Name of path to control file (see details). Typically, this file does not yet normally exist, but will house the code code for this run.

Details

Note that `text` can contain an `"{run_id}"` string. E.g. "Models/run{run_id}.mod" will use the name "Models/runm1.mod" if `run_id(m1)` is "m1".

Value

`character` with path to NONMEM control file to be copied immediately prior to running (with `run_nm()`).

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

ctl_name(m1)
ctl_path(m1)
```
data_path

m1 <- m1 %>% ctl_path("Models/nm_{run_id}.ctl")
ctl_path(m1)

---

data_path  
Get/set path to dataset

Description

[Stable]
Mainly used to associate a dataset with an nm object. Requires ctl_contents to already be specified.

Usage

data_path(m, text)

Arguments

m
An nm object.
text
Optional character. Path to input dataset.

Value

if text is not specified, will return the data_path name otherwise will return an nm object with modified data_path field.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

data_path(m1) ## display data name
**decision**

Make decision point

**Description**

*Experimental*

Formalise process of decision making. Creates a decision point in the workflow where subsequent parts of your workflow depend on this decision, e.g. if you compare a 1 compartment and 2 compartment and decide based on the OFV and goodness of fit plots that the 1 compartment model is better and subsequent steps will build off of this, it is worth putting a decision point in your code so that if you are to rerun the workflow with a new/updated dataset, the decision can be revisited prior to moving onto the parts of the workflow that depend on the 1 compartment decision. The function requests inputs (values and files) that you base a decision on and stop for users to remake decision if inputs change.

**Usage**

```r
decision(
  inputs = c(),
  file_inputs = c(),
  auto = logical(),
  outcome = character(),
  force = FALSE
)
```

**Arguments**

- `inputs` Optional non file names upon which decision depends.
- `file_inputs` Optional file names upon which decision depends.
- `auto` Optional logical. logical statement for automatic decisions.
- `outcome` Character. Description of the decision outcome.
- `force` Logical (default = FALSE). Force a stop in the workflow so decision has been remade.

**Details**

There are two ways to use decision:

**Automatic:** An auto decision (see examples below) works like `stopifnot()`. It requires a logical (TRUE/FALSE) condition. Doing this this way ensures that creates fewer points in your workflow where at the cost of removing. If updating a workflow (e.g. with an updated dataset), so long as the TRUE/FALSE is TRUE, the workflow will proceed uninterrupted. If the condition flips to FALSE the workflow will stop as it will be assumed that subsequent steps will no longer be valid.
Manual: Requires specification of either input or file_inputs (or both) AND outcome. Inputs represent information you have considered in your decision and outcome is a text description of the resulting decision. The assumption made is that if inputs have not changed since the last decision was made.

Value

No return value, called for side effects.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))
m2 <- m1 %>% child("m2")
m2WT <- m1 %>% child("m2WT")

## Not run:
if(interactive()){  
## a decision based on summary statistics
decision(
  inputs = summary_wide(c(m1, m2, m2WT)),
  outcome = "m1 is better"
) # next line must be end of chunk

## a decision based also on goodness of fit plots
decision(
  inputs = summary_wide(c(m1, m2, m2WT)),
  file_inputs = c(
    "Results/basic_gof.m1.nb.html",
    "Results/basic_gof.m2.nb.html"
  ),
  outcome = "m1 is better"
) # next line must be end of chunk

## a decision based on an automatic TRUE/FALSE criteria
## here we're ensuring m1 has the lowest AIC
decision(auto = (AIC(m1) == min(AIC(m1, m2, m3))))
}

## End(Not run)
```
delete_dollar | Delete a NONMEM subroutine from control file contents

Description

[Stable]

Usage

delete_dollar(m, dollar)

Arguments

m An nm object.
dollar Character. Name of subroutine.

Value

An nm object with modified ctl_contents field.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("TABLE")
m1 <- m1 %>% delete_dollar("TABLE")
m1 %>% dollar("TABLE")  ## missing

dollar | Get/set existing subroutine

Description

[Stable]

The fast way to see the contents of a particular subroutine directly in the R console. It can also be used to set the contents of a NONMEM subroutine in place of manual edits.

Usage

dollar(m, dollar, ..., add_dollar_text = TRUE)
Arguments

m  An nm object.
dollar  Character. Name of NONMEM subroutine to target.
...  Additional arguments to be passed to text(). If specified these will set the contents of the subroutine. See examples below.
add_dollar_text  Logical (default = TRUE). Should the $XXXX string be added to text.

Value

If dollar is specified returns the relevant subroutine of the control file as a character. Otherwise returns an nm object with modified ctl_contents field.

See Also

insert_dollar(), delete_dollar()

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("PK")  ## displays existing $PK
m1 %>% dollar("THETA")
c(m1, m1) %>% dollar("THETA")  # display $THETAs for multiple NONMEM runs
Usage

advan(m, text)
trans(m, text)
tol(m, text)

Arguments

m  An nm object.
text  Optional number/character number to set to.

Value

If text is specified returns an nm object with modified ctl_contents field. Otherwise returns the value of the advan, trans, or tol.

See Also

subroutine()

exclude_rows  Exclude rows of NONMEM dataset

Description

[Stable]

A mechanism for excluding outliers during data cleaning. Create exploratory plots, identify rows of the dataset to be considered outliers for exclusion, and then feed that filtered dataset into this function to exclude them from the dataset. Requires a corresponding IGNORE statement - see argument descriptions for more details.

Usage

exclude_rows(d, dexcl, exclude_col = "EXCL")

Arguments

d  A data.frame for containing the full NONMEM dataset. Should contain a column for identifying excluded rows named with the exclude_col argument.
dexcl  A smaller data.frame consisting of rows to be ignored. Need not contain all columns of d but each column should be present in d.
exclude_col  Character (default = "EXCL"). Name of a binary exclude column in d. This should be accompanied with a IGNORE=(EXCL.GT.0) statement in $DATA.
Value

A modified version of d with exclude_col set to 1 for rows coinciding with dexcl.

See Also

read_derived_data(), write_derived_data()

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

d <- input_data(m1)
d$EXCL <- 0 ## start with no rows excluded

## use with dplyr
dexcl <- d %>%
    dplyr::filter(ID == 6, TIME > 3) %>%
    dplyr::select(ID, TIME, DV, EXCL)
dexcl ## view rows to be excluded

d <- d %>% exclude_rows(dexcl)

d %>% dplyr::filter(ID %in% 6)
```

Description

[Stable]

Uses dataset to automatically fill $INPUT in control file.

Usage

fill_input(m, ...)

Arguments

- **m**: An nm object.
- **...**: Either keep, drop, or rename arguments. See examples.
Details

If a new dataset with different columns is assigned to an nm object, $INPUT will not be correct and so it may necessary to apply fill_input() again.

See examples for how to use drop and rename arguments to control how $INPUT is written.

Value

An nm object with modified ctl_contents field.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
               based_on = file.path(exdir, "Models", "ADVAN2.mod"),
               data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("INPUT") ## shows placeholder for column names

m1 <- m1 %>% fill_input()
m1 %>% dollar("INPUT") ## view $INPUT

## following will will drop the "RATE" column
m1 <- m1 %>% fill_input(drop = "RATE")
## no RATE column so will not drop anything
m1 %>% dollar("INPUT")

## following will rename "DATE" to be "DAT0"
m1 <- m1 %>% fill_input(rename = c("DAT0" = "DATE"))
## no DATE column so will not rename anything
m1 %>% dollar("INPUT") ## view $INPUT
```

---

**find_nonmem**  

*Find location of NONMEM installation*

Description

[Experimental]

Attempts to find location of NONMEM installation directory used by PsN. Can be useful for finding the location of parafiles etc.

Usage

```r
find_nm_install_path(name = "default")

find_nm_tran_path(name = "default", warn = TRUE)
```
Arguments

name Character name of NONMEM installation (according to PsN).
warn Logical (default = TRUE) to warn if fails to find NMTRAN.exe.

Details

The function `find_nm_install_path()` will attempt to use a locally available PsN installation to get this information. If the PsN installation is on a remote server, this function will not work (it will return a NULL).

The function `find_nm_tran_path()` will attempt to use a locally available PsN installation to get this information. If the PsN installation is on a remote server, this function will not work (it will return a NULL). This is normally used to set `nm_tran_command()`. If this function cannot find installation, you will need to set `nm_tran_command()`, manually.

Value

If functions cannot find installation they will return NULL without errors or warning, otherwise they will return the located paths.

See Also

nm_tran_command()

---

gsub_ctl Pattern replacement for control file contents

Description

[Stable]

A wrapper around gsub so that control files may be modified using gsub syntax. Can be useful for simple find replace operations in a control stream. Ensure you use the "view diff" app afterwards to make sure the find replace proceeded as intended.

Usage

```r
gsub_ctl(m, pattern, replacement, ..., dollar = NA_character_)
```

Arguments

- `m` An nm object.
- `pattern` Argument passed to gsub().
- `replacement` Argument passed to gsub().
- `...` Additional arguments passed to gsub().
- `dollar` Character name of subroutine.
Value

An nm object with modified ctl_contents field.

See Also

apply_manual_edit()

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("EST")

m1 <- m1 %>% gsub_ctl("ISAMPLE=300", "ISAMPLE=600")

m1 %>% dollar("EST")

Description

[Stable]

Usage

ignore(ctl, ignore_char)

Arguments

ctl An nm object.
ignore_char Optional character. Ignore statement to set in $DATA.

Value

If ignore_char is specified returns an nm object with modified ctl_contents field. If no IGNORE present, returns FALSE. Otherwise returns the value of the IGNORE statement in $DATA.

See Also

data_ignore_char(), data_filter_char()
import

import staged files into project

Description

[Stable]

This function is used by the "code library" RStudio 'Addin' to bring external code into your project.

Usage

import(
  copy_table,  # A data frame or character. if data.frame should be output from stage(), if character path, result will be stage()d first.
  overwrite = FALSE,  # Logical (default = FALSE).
  silent = FALSE,  # Logical (default = FALSE).
  skip = "\.mod$",  # Character (default = "\.mod$"). Pattern to skip. Model files will be imported directly into the project in order to avoid conflicts and will instead reside only in the staging area.
  find_replace_dir_names = TRUE  # Logical (default = TRUE). Will attempt to find replace strings in scripts to reflect nm_default_dirs().
)

Arguments

copy_table
overwrite
silent
skip
find_replace_dir_names
init_theta

Get/set initial parameters

Description

[Stable]
These functions are useful to obtain and modify initial values of $THETA, $OMEGA and $SIGMA.

Usage

init_theta(m, replace, ...)
init_omega(m, replace, ...)
init_sigma(m, replace, ...)

Arguments

- `m`: An nm object.
- `replace`: Optional tibble for replacement.
- `...`: Additional arguments for mutating initial estimate NONMEM subroutines. See examples.

Examples

```r
## requires NMproject directory structure
## Not run:
## both of these following operations are easier in the shiny code library
## RStudio 'Addin'.

ls_code_library("Models/ADVAN2.mod") %>%
  import() ## ends up in "staging/Models"

ls_code_library("Scripts/AUC.R") %>%
  import() ## ends up "scripts" directory

## End(Not run)
```
**Details**

It’s easiest to learn this function by view examples, the vignette and the demo `setup_nm_demo()`. It is a good idea to view the resulting `data.frame` to see the columns that are able to be manipulated.

**Value**

If `replace` is specified returns an `nm` object with modified `ctl_contents` field. Otherwise returns a `tibble` or list of `tibbles` with initial estimation information.

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 <- m1 %>%
     fill_input() %>%
     init_theta(init = c(-2, 0.5, 1)) %>%
     init_sigma(init = c(0.1, 0.1)) # %%
# run_nm()

init_theta(m1) ## display current $THETA in tibble-form
init_omega(m1) ## display current $OMEGA in tibble-form

## here we supply a named vector in a different order
m1 <- m1 %>%
     init_theta(init = c(KA = -2, V = 1))

m1 %>% dollar("THETA")

## can also manipulate other aspects (like the FIX column) similarly
m1 <- m1 %>%
     init_theta(init = c(KA = -2, V = 1),
                FIX = c(KA = TRUE))

m1 %>% dollar("THETA")

## perturb all parameters by ~10%
m1 <- m1 %>%
     init_theta(init = rnorm(length(init), mean = init, sd = 0.1))

m1 %>% dollar("THETA")
```
**Description**

[Stable]

Uses `data_path` field of object to locate data and read in.

**Usage**

```r
input_data(m, filter = FALSE, na = ".", ...)
```

**Arguments**

- `m` An `nm` object.
- `filter` Logical (default = FALSE). Applies NONMEM ignore statement to filter dataset.
- `na` Character. Passed to `utils::read.csv()`
- `...` Additional arguments passed to either `read_derived_data()` (if `write_derived_data()` was used to create derived dataset) or `utils::read.csv()`

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

d <- input_data(m1)
head(d)

## only non-ignored rows
d_nonignore <- input_data(m1, filter = TRUE)
```

---

**insert_dollar**

`Insert a new subroutine into control file_contents`

**Description**

[Stable]

Mostly a back end function used by other functions.

**Usage**

```r
insert_dollar(m, dollar, text, after_dollar)
```
is_finished

Arguments

- **m**: An nm object.
- **dollar**: Character. Name of subroutine to insert.
- **text**: Character vector. Text to fill.
- **after_dollar**: Character name of preceding subroutine. The new subroutine will be inserted immediately after it.

Value

An nm object with modified ctl_contents field.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 <- m1 %>% insert_dollar("MODEL", "$MODEL
  COMP = (CENTRAL)
  ", after_dollar = "SUB")

m1 %>% dollar("MODEL")
```

is_finished

Tests if job is finished

Description

[Stable]

Usage

```r
is_finished(r, initial_timeout = NA)
```

Arguments

- **r**: An nm object.
- **initial_timeout**: Deprecated. See `wait_finish()`.

Value

A logical vector with TRUE or FALSE values.
Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

is_finished(m1) # FALSE
```

---

**is_nm**

Test if object is an nm coercible object

---

**Description**

[Stable]

Mostly internal functions to test object types.

**Usage**

```r
is_nm_list(x)

is_nm_generic(x)
```

**Arguments**

- `x` Object.

**Value**

A logical vector with TRUE or FALSE values.

---

**is_nmproject_dir**

Is the directory an NMproject directory

---

**Description**

[Stable]

Find out whether current (or specified) directory is an NMproject directory or not.

**Usage**

```r
is_nmproject_dir(path = getwd())
```
Arguments

path  
Optional path to test if it’s an NMproject or not.

Value

Logical TRUE or FALSE

Description

[Experimental]

Usage

is_successful(r)

Arguments

r  
An nm object.

Value

TRUE if run was successful, FALSE otherwise.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

is_successful(m1) ## FALSE
job_stats  

Get job stats for a completed NONMEM run

Description

[Experimental]  
Gets attributes of the run like run time, queue time.

Usage

job_stats(m)

Arguments

m  
An nm object.

Value

A wide format tibble with information about the job execution times.

Examples

## Below code requires NONMEM to be installed
## Not run:

#' # create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

dc <- tibble(cores = c(1, 3, 10, 30)) %>%
  mutate(m = m1) %>%
  child(run_id = cores) %>%
  run_in("Models/m1_coretest") %>%
  cmd("execute {ctl_name} -parafile={parafile} -dir={run_dir} -nodes={cores}"") %>%
  parafile("/opt/NONMEM/nm75/run/mpilinux8.pnm") %>%
  cores(cores))

dc$m %>% cmd()

dc$m %>%
  run_nm() %>%
  wait_finish()

## extract job statistics and plot cores vs Rtime or Ttime
## to get plots of run time and total time vs number of CPUs
ls_code_library

```r
dc$m %>%
  job_stats() %>%
  ggplot(aes(x = cores, y = Rtime)) +
  theme_bw() +
  geom_point()
## End(Not run)
```

---

**ls_code_library**  
*List files in code library*

**Description**

[Stable]

A low level function to interact with the code library. It is easier in most cases to use the shiny "code library" RStudio 'Addin'.

**Usage**

```r
ls_code_library(pattern = ".")
```

**Arguments**

- `pattern`  
  Optional character. Filter the code library use regex.

**Value**

Character vector of matched file paths.

**See Also**

`code_library()`, `stage()`, `import()`

**Examples**

```r
ls_code_library("Models/ADVAN2.mod")
```

## requires NMproject directory structure to operate in
## Not run:
```r
ls_code_library("Models/ADVAN2.mod") %>%
  stage()
## End(Not run)
```
**ls_scripts**  
*List scripts*

**Description**

[Stable]

**Usage**

```r
ls_scripts(folder = ".", extn = "r|R|Rmd|rmd", recursive = TRUE)
```

**Arguments**

- `folder`  
  String describing folder to search recursively in.

- `extn`  
  Character (can be regex) giving extension to limit search to.

- `recursive`  
  Logical (default = TRUE). Should directories be searched recursively.

**Value**

Character vector of matched file paths.

**Examples**

```r
## find all scripts with the string "AUC("
ls_scripts("~/path/to/analysis/Scripts") %>% search_raw("AUC\(")
```

**make_boot_datasets**  
*Prepare a bootstrap tibble*

**Description**

[Stable]

Creates bootstrap datasets and returns corresponding nn objects. Requires the necessary rsample splitting objects to be present. See examples.

**Usage**

```r
make_boot_datasets(
  m,
  samples = 10,
  data_folder = file.path(nm_dir("derived_data"), "bootstrap_datasets"),
  overwrite = FALSE,
  id_var = "ID",
  ...
)
```
make_boot_datasets

Arguments

- **m**: An nm object.
- **samples**: Number of samples.
- **data_folder**: Folder (relative path) to store datasets.
- **overwrite**: Logical (default = FALSE). Overwrites previous files.
- **id_var**: Character (default = "ID"). Name of ID column in dataset.
- ... Arguments passed to `fill_input()`.

Value

A tibble with `samples` rows and an nm object object column `m` for execution of the bootstrap.

Examples

```r
## The following only works inside an NMproject directory structure and
## and requires NONMEM installed
## Not run:
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))
d <- input_data(m1)
## in your dataset production script
d <- d %>%
    mutate(
        WT_C = cut(WT, breaks = 2, labels = FALSE),
        STRATA = paste(SEX, WT_C, sep = "_")
    )
d_id <- d %>% distinct(ID, STRATA)
set.seed(123)
## create large set of resamples (to enable simulation to grow
## without ruining seed)
bootsplits <- rsample::bootstraps(d_id, 100, strata = "STRATA")
dir.create("DerivedData", showWarnings = FALSE)
bootsplits %>% saveRDS("DerivedData/bootsplit_data.csv.RData")
## In a model development script, the following, performs a
## 100 sample bootstrap of model m1
m1_boot <- m1 %>% make_boot_datasets(samples = 100, overwrite = TRUE)
```
make_OCC_every_dose

Description

[Experimental]

Creates an OCC column that increments in accordance to specified condition. To be used in a
dplyr::mutate() statement dplyr::group_by()'s by "ID".

Usage

make_OCC_every_dose(d, dose_trigger, new_OCC_trigger)

Arguments

d        A data.frame. NONMEM ready input dataset.
dose_trigger Logical expression for defining a dosing row.
new_OCC_trigger Logical expression for defining when OCC should increment.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))
d <- input_data(m1)

## OCC increments on every dosing interval with more than 4 samples
d %>% make_OCC_every_dose(!is.na(AMT), any(!is.na(DV)))
**make_xv_datasets**

Write (bootstrap) cross validation datasets

---

**Description**

*[Experimental]*

Similar to `make_boot_datasets()`, but sets up "out of bag" datasets for model evaluation.

**Usage**

```r
make_xv_datasets(
  dboot,
  data_folder = file.path(nm_dir("derived_data"), "bootstrap_datasets"),
  overwrite = FALSE,
  id_var = "ID"
)
```

**Arguments**

- `dboot`: Output from `make_boot_datasets()`.
- `data_folder`: Folder to store datasets.
- `overwrite`: Logical. Overwrite previous files or not.
- `id_var`: Character (default = "ID"). Name of ID column.

**Value**

A tibble of nm objects similar to `make_boot_datasets()` output.

---

**new_nm**

Create a new (parent) nm object

---

**Description**

*[Stable]*

Create a new parent nm object. Normally the first NONMEM object you create will be using this function. Subsequent objects created with the `child()` function will inherit the properties of the parent run.

**Usage**

```r
ew_nm(based_on, run_id = NA_character_, data_path, cmd, force = FALSE)
```
Arguments

- **based_on** Character. Relative path to an existing control file from which to base this run. NMproject will not modify or run this control file. Instead it will create a new control file specified by the `ctl_name` field (see Details below).

- **run_id** Character. Run identifier. This is used to name the run and output files such as $TABLE outputs.

- **data_path** Character. Path to dataset. If this is not specified, NMproject will try to guess based on the current $DATA components of the file specified in `based_on`. However, it is recommended to specify this explicitly as a relative path.

- **cmd** Optional character. PsN command to use. If unspecified will use `getOption("nm_default_fields")` value of `cmd`. Use glue notation for inheritance. See details.

- **force** (Default = FALSE). Forces object creation even if `based_on` model is in the `nm_dir("models")` directory.

Details

The `cmd` field uses glue notation. So instead of specifying execute `runm1.mod -dir=m1`, it is best to specify execute `{ctl_name} -dir={run_dir}`. The values of `ctl_name` and `run_dir` refer to object fields and if these change value like when the `child()` function is used to create a separate child object, the `cmd` field will update automatically.

Value

An object of class `nm_list`. Attributes can be viewed by printing the object in the console.

Object fields

Each field has a corresponding function (documented in `nm_getsetters`) of the same name to access and modify its value.

- **type** The PsN run type. Default is execute.
- **run_id** The run identifier. E.g. m1.
- **run_in** The directory to copy control files and run NONMEM. Default = "Models".
- **executed** For internal use.
- **ctl_contents** Stores the contents of the control file to be written to disk when the `run_nm()` function is used on the object.
- **data_path** Path to the NONMEM ready dataset (from base project directory).
- **cmd** See details above.
- **cores** Numbers of cores to use. Requires a `cmd` value that uses the `{cores}` glue field.
- **run_dir** PsN directory to run the NONMEM run. Default is to be the same as the `run_id` for simplicity.
- **results_dir** Location to store results files from diagnostic reports executed with `nm_render()`.
- **unique_id** For internal use.
- **lst_path** Normally does not require setting. Path to the expected .lst file.
See Also

`nm_getsetters()`, `child()`

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 ## display object fields
cmd(m1)
ctl_name(m1)
run_dir(m1)
```

Description

[Experimental]

`nmsave_plot` is a wrapper around `ggplot2::ggsave()` for nm objects, `nmsave_table` is a wrapper for saving data.frames to file in the form of a .csv file.

Usage

```r
nmsave_plot(
  r, 
  object, 
  file_name, 
  directory = results_dir(r), 
  width = 7, 
  height = 5, 
  dpi = 300, 
  ...
)
```

```r
nmsave_table(r, object, file_name, directory = results_dir(r), ...)```

Arguments

- `r` An nm object.
- `object` A list of plotting objects.
- `file_name` Character. Name of results file.
nm_create_analysis_project

Create analysis project

Description

[stable] This is the underlying function used by: File -> New Project -> New Directory -> New NMproject. It creates a new analysis working directory with a directory structure similar to an R package.

Usage

nm_create_analysis_project(
  path,
  dirs = nm_default_dirs(),
  style = c("analysis", "analysis-package"),
  use_renv = FALSE,
  readme_template_package = "NMproject",
  ...
)

Arguments

path Character path (relative or absolute) to project. If just specifying a name, this will create the analysis project in the current working directory. See details for naming requirements.
dirs Character list or vector. Default = nm_default_dirs(). Can also handle an ordered string which is supplied by the RStudio project template interface.
style Character. Either "analysis" or "analysis-package" See details for path requirements and function behaviour.
use_renv Logical (default = FALSE). Should renv be used or not in project.
readme_template_package Package name from which to load the README template (default = "NMproject")

... Deprecated.
Details

The function works like as is inspired by starters::create_analysis_project(). There is no restriction on directory name. It is therefore possible to violate R package naming conventions.

When style = "analysis" is selected, the analysis directory will be package-like in structure, with the package name "localanalysis". For style = "analysis-package", path should contain only (ASCII) letters, numbers and dot, have at least two characters and start with a letter and not end in a dot. See Description file requirements for more information.

This is to cater to users who like underscores and aren’t interested in creating a package.

Default modelling directories

Default modelling directories can be modified with nm_default_dirs option (see options() for information on how to modify this). A (partially) named list of directories to be used by nm_create_analysis_project. Required names are "models", "scripts" and "results". By default these are set to "Models", "Scripts" and "Results", respectively. Additional nameless characters (e.g. "SourceData") correspond to additional modelling directories.

"SourceData": intended for unmodified source datasets entering the analysis project.
"DerivedData": intended for cleaned and processed NONMEM ready datasets
"Scripts": intended for all R scripts
"Models": intended for all NONMEM modelling
"Results": intended as default location for run diagnostics, plots and tables

See Also

nm_default_dirs() for modifying default directory structure.

---

**nm_default_dir**

Get a default directory

Description

[Deprecated]

Get subdirectory (relative) paths in a configuration independent way. The configuration can be modified with nm_default_dirs(). Can be useful in scripts, where you need to refer to locations of model files or output files.

Usage

nm_default_dir(name = c("scripts", "models", "results"), ...)

Arguments

name

Character. Directory type. Should be either "scripts", "models" or "results".

...  

Deprecated.
nm_default_dirs

Setup analysis subdirectories

Description

[Stable]
This allows organisations/individuals with their own directory to customize their directory structure

Usage

nm_default_dirs(dir_list)

Arguments

dir_list Optional named list or vector. Names "scripts" and "models" must be present. The rest can be unnamed.

Value

if dir_list is missing, will return value of getOption("nm_default_dirs") otherwise will set option nm_default_dirs.

Examples

orig_list <- nm_default_dirs()
orig_list

nm_default_dirs(list(
  models = "Models",
  scripts = "Scripts",
  results = "Results",
  source_data = "SourceData",
  derived_data = "Data"
))

nm_default_dirs()
nm_default_dirs(orig_list)
**nm_default_fields**

Setup default nm object fields

**Description**

[Stable]

This allows organisations/individuals with their own nm object field preferences to set these.

**Usage**

\texttt{nm_default_fields(field_list)}

**Arguments**

- \texttt{field_list} Optional named list or vector. Names correspond to function names and object fields, values correspond to what will be set.

**Value**

If \texttt{field_list} is missing, will return value of \texttt{getOption("nm_default_fields")}, otherwise will set option \texttt{nm_default_fields}.

**Examples**

\begin{verbatim}
  nm_default_fields()
  nm_default_fields(list(
    cmd = "execute {ctl_name} -dir={run_dir}"
  ))
  nm_default_fields()
\end{verbatim}

**nm_diff**

Compute diff between two NONMEM runs

**Description**

[Stable]

The easiest way to use this function is via the "view diff" RStudio 'Addin'.

NMproject's control file manipulation functions (e.g. \texttt{subroutine()}) may not work for all control files. It is the responsibility of the user to check automatic manipulations are done properly. Displaying diffs provides a means of manually checking what was done.

**Usage**

\texttt{nm_diff(m, ref_m, format = "raw")}
Arguments

- **m**: An `nm` object.
- **ref_m**: An optional `nm` object (base/reference object). If not specified, it will compute the diff the initial control file contents associated with the object at the time of object create. This information is stored in the `ctl_orig` field.
- **format**: Character (default = "raw") argument passed to `diffobj::diffChr()`.

Value

Invisibly returns a character vector of the diff.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1", 
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m2 <- m1 %>%
  child(run_id = "m2") %>%
  subroutine(advan = 2, trans = 2)

nm_diff(m2, m1)
```

---

### nm_dir

*Get a directory name*

**Description**

[Stable]

Get subdirectory (relative) paths in a configuration independent way. The configuration can be modified with `nm_default_dirs()`. Can be useful in scripts, where you need to refer to locations of model files or output files.

**Usage**

`nm_dir(name, ...)`

**Arguments**

- **name**: Character. Directory type. Should be either "scripts", "models" or "results".
- **...**: Deprecated.

**See Also**

`nm_default_dirs()`
Examples

nm_dir("scripts") ## will return the path to the "scripts" directory
nm_dir("models")
nm_dir("results")

nm_getsetters

Functions to access and modify fields of nm objects

Description

[Stable]

The fields of an object can be viewed by printing the object. Each field has a corresponding function of the same name to access and modify its value.

Usage

run_dir(m, text)
cmd(m, text)
type(m, text)
parent_run_id(m, text)
parent_run_in(m, text)
parent_ctl_name(m, text)
parent_results_dir(m, text)
unique_id(m, text)
ctl_name(m, text)
results_dir(m, text)
run_in(m, text)
run_id(m, text)
result_files(m, text)
lst_path(m, text)
Arguments

m
An nm object.

text
Optional character for replacing field. If present function will modify field (of same name as function) otherwise will return value of field (of same name as function).

Details

Easiest way to see all fields of an object is to type the object into the console and hit enter. This will display the value of each field.

The fundamental structure of all these functions is the same:
To access the value of a field: `m %>% fieldname()` or equivalently `fieldname(m)`.
To modify the value of a field: `m <- m %>% fieldname("newvalue")`

Some fields like `cmd` are glue fields. In these cases inserting expressions inside braces in `text` will evaluate the expression (see examples).

Value

The value of the specified field of `m` if `text` is missing. Otherwise an nm object with modified field.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

run_dir(m1)

m1 <- m1 %>% run_dir("[run_id]_dir")
run_dir(m1)

## set cmd field of m1
m1 <- m1 %>% cmd("execute {ctl_name} -dir={run_dir}"

m1 %>% cmd()
## displays "execute runm1.mod -dir=m1"

## can also view field when viewing object
m1
```
nm_getsetters_execution

Execution related functions to access and modify fields of nm objects

Description

[Stable]
The fields of an object can be viewed by printing the object. Each field has a corresponding function of the same name to access and modify it’s value.

Usage

cores(m, text)
paraf(m, text)
walltime(m, text)
executed(m, text)

Arguments

m An nm object.
text Optional character for replacing field. If present function will modify field (of same name as function) otherwise will return value of field (of same name as function).

Details

Easiest way to see all fields of an object is to type the object into the console and hit enter. This will display the value of each field. some fields like cmd are glue fields. In these cases inserting expressions inside braces in text will evaluate the expression.

The fundamental structure of all these functions is the same:
To access the value of a field: m %>% fieldname() or equivalently fieldname(m)
To modify the value of a field: m <- m %>% fieldname("newvalue")

Examples

# create example object ml from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
ml <- new_nm(run_id = "ml",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

ml <- ml %>% cmd("execute -paraf={paraf} {ctl_name} -dir={run_dir} -nodes={cores}"")
nm_list_gather

Get all nm_list objects

Description

[Stable]

Get all nm objects in an environment. By default this is the global workspace.

Usage

nm_list_gather(x = .GlobalEnv)

Arguments

x

An environment (default = .GlobalEnv) to search or data.frame with (nm_list
column) or nm_list.

Value

A single nm_list object with all model objects in environment x.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m2 <- m1 %>% child("m2")

m_all <- nm_list_gather()

identical(
    m_all %>% subset(run_id(m_all) %in% "m1"),
    m1
)
### nm_output_path

**Find an output file associated with a run**

**Description**

[Stable]

This is primarily a backend function used to identify output file paths associated with nm objects.

**Usage**

```r
nm_output_path(m, extn, file_name)
```

**Arguments**

- `m`  
  An nm object.

- `extn`  
  Character. Name of extension.

- `file_name`  
  Optional character. Name of file name.

**Value**

The path to the relevant output file of `m`.

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1", 
              based_on = file.path(exdir, "Models", "ADVAN2.mod"), 
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% nm_output_path("ext") ## path to ext file
```

### nm_read_table

**Fast read of NONMEM output table**

**Description**

[Stable]

Reads in $TABLE outputs rapidly. `output_table()` is a higher level function for reading output files and combining with input datasets.

**Usage**

```r
nm_read_table(file, ...)
```
Arguments

file  File argument from utils::read.table().

... Other arguments to be passed to utils::read.table().

Value

A data.frame from a relevant $TABLE output file.

See Also

output_table()

-----------------------------------------------------------------

nm_render  Create run reports

-----------------------------------------------------------------

Description

[Stable]

A wrapper around rmarkdown::render for nm objects. Use markdown templates to create a customised set of diagnostics to reuse on multiple models. In the demo an example is shown in Scripts/basic_gof.Rmd, but ideally you’ll create your own customised version with everything you need to evaluate your model. To create an R markdown diagnostic template go to FILE -> New File -> R markdown -> From Template the select from one of the following:

- model diagnostic
- VPC diagnostic
- PPC diagnostic
- bootstrap results (nm_list_render)

These are intentionally minimal templates that can be run as notebooks or as automated diagnostics run with nm_render. Follow the instructions at the top of the template for more details.

Usage

nm_render(
  m,
  input,
  output_file = NA,
  args = list(),
  force = getOption("nm.force_render"),
  async = FALSE,
  ...
)

nm_list_render(
  m,
Arguments

m  An nm object.
input  Character. Same as rmarkdown::render() arg.
output_file  Character. Same as rmarkdown::render() arg.
args  List. Same as "params" arg in rmarkdown::render().
force  Logical (default = getOption("nm.force_render")). Will force execution.
async  Experimental option to use future package.
...  Additional argument passed to rmarkdown::render().

Details

input must refer to a properly specified Rmd document. The R markdown template "model diagnostic" in RStudio sets this up for you.

These R markdown templates are usable as R Notebooks (e.g. for code development and debugging) if the object .m is defined in the global work space first.

nm_list_render() is mostly used for bootstraps, and other routines where a parent run spawns multiple children in the form of an nm_list.

Value

The same nm object, m, with modified results_files field.

Examples

## requires NONMEM to be installed
## Not run:
m1 %>% nm_render("Scripts/basic_gof.Rmd")

## to run "Scripts/basic_gof.Rmd" as an R Notebook
## first define .m

.m <- m1 ## Now you can run "Scripts/basic_gof.Rmd" as a Notebook

## End(Not run)
Description

[Stable]
Get wide (or a long) tibble showing summary results.

Usage

summary_wide(
  ...
  include_fields = character(),
  parameters = c("none", "new", "all"),
  m = TRUE,
  trans = TRUE
)

summary_long(..., parameters = c("none", "new", "all"))

Arguments

... Arguments passed to summary(), usually a vector of nm object + options.
include_fields Character vector of nm object fields to include as columns in the output. Default is empty.
parameters Character. Either "none" (default), "new", or "all" indicating whether parameter values should be included in the summary tibble. Specifying "new" means that only parameters that aren’t in the parent run are included in outputs. This is useful if wanting to know the value of an added parameter but not all the parameters (e.g. in a covariate analysis).
m Logical (default = TRUE). Should model object be included as the m column.
trans Logical (default = TRUE). Should parameters be transformed in accordance with $THETA/$OMEGA/$SIGMA comments. This is only valid if parameters is "new" or "all.

Value

A wide format tibble with run results.
A long format tibble with run results coerced to character form.

Examples

## requires NONMEM to be installed

## Not run:
nm_tran

Run NMTRAN step of a NONMEM job

Description

[Stable]
This is the function behind the "nm_tran" RStudio 'Addin', which is the recommended way to use this functionality. Highlight your code (e.g see examples below for a code segment), and then open the "nm_tran" RStudio 'Addin'.
Useful especially on grid infrastructures where it may take a while for NONMEM to start return control file and dataset errors. Runs initial NMTRAN step of NONMEM in a temporary directory where control file and dataset checks are performed. Stops before running NONMEM.

Usage

nm_tran(x)

Arguments

x            An nm object.

Value

The same x object is returned, called for side effects.

See Also

run_nm(), nm_tran_command() for configuration.

Examples

## requires NONMEM to be installed
## Not run:
## highlight the code below and use the "nm_tran" RStudio 'Addin'

m1 <- new_nm(run_id = "m1",
             based_on = "staging/ Models/ADVAN2.mod",
             summary_wide(c(m1, m2))
summary_long(c(m1, m2))

## End(Not run)
```r

```}

---

**nm_tran_command**

Get/set nm_tran_command

**Description**

[Stable]

The function `nm_tran()` needs the location of NMTRAN.exe to function. This is guessed at package load, assuming PsN is on the $PATH environmental variable. If this is not the case, then you can manually set the path and command used.

**Usage**

```r
nm_tran_command(text)
```

**Arguments**

- `text` Optional character. If specified will set nm_tran_command otherwise it will display the current option value.

**Details**

text can just be the path to NMTRAN.exe in which case nm_tran_command will use the format /path/to/NMTRAN.exe < {ctl_name} to launch NMTRAN.exe where {ctl_name} is the name of the control file. Specifying

```r
nm_tran_command("/path/to/NMTRAN.exe < {ctl_name}"")
```

is equivalent to:

```r
nm_tran_command("/path/to/NMTRAN.exe")
```

More complicated formats are possible with different installations which can be seen examples.

As with all NMproject configuration options set this up either at the beginning of your script, in your .Rprofile or for all users in Rprofile.site. See FAQ for setting up configuration options permanently.

**Value**

If text is missing will get and return the current NMTRAN command.

**See Also**

`find_nm_tran_path()`, `nm_tran()`
Examples

```r
orig_cmd <- nm_tran_command()
orig_cmd

# the following two are equivalent
nm_tran_command("/opt/NONMEM/nm75/tr/NMTRAN.exe")
nm_tran_command()

nm_tran_command("/opt/NONMEM/nm75/tr/NMTRAN.exe < {ctl_name}"")
nm_tran_command()

nm_tran_command(orig_cmd)
```

---

**nm_tree**  
*Make data.tree object*

---

**Description**

*Experimental*

Draw a tree diagram showing model development path.

**Usage**

```r
nm_tree(..., summary = FALSE)
```

**Arguments**

- `...`  
  Arguments passed to `nm_list_gather()`.
- `summary`  
  Logical (default = FALSE). Should `summary_wide()` variables be appended.

**Value**

A `data.tree` object.

---

**NONMEM_version**  
*NONMEM version info*

---

**Description**

*Stable*

Gets version information about the NONMEM installation, PsN installation and compilers. Can be useful for documentation purposes.
Usage

NONMEM_version()

Value

Returns list with version info for NONMEM, PsN, perl and fortran compiler (only gfortran currently).

Get Objective Function Value (OFV)

Description

[Stable]

Extracts OFV from .ext file.

Usage

ofv(r)

Arguments

r An nm object.

Value

The numeric value of the OFV.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

is_finished(m1) ## FALSE until run is completed
ofv(m1) ## NA until m1 is finished
**omega_matrix** *Get OMEGA matrix from run*

**Description**

[Experimental]

Obtain in matrix form the OMEGA matrix. This is primarily to feed into other packages such as mrgsolve.

**Usage**

`omega_matrix(r)`

**Arguments**

- `r` An nm object.

**Value**

A matrix object.

**Examples**

```r
## requires NONMEM to be installed
## Not run:
## matrix of initial estimates
m1 %>% omega_matrix()

## matrix of final estimates
m1 %>% update_parameters() %>%
    omega_matrix()

## End(Not run)
```

**output_table** *Reads all $TABLE outputs and merge with input dataset*

**Description**

[Stable]

Produces a single merged output dataset will all columns of $INPUT dataset. This is useful for reuse of exploratory data plots as diagnostic plots as all columns including text columns used for ggplot facetting will be present.
Usage

output_table(r, only_append = c(), ...)

output_table_first(r, ...)

Arguments

r
An object of class nm.

only_append
Optional character vector. If missing will append all, otherwise will append only those variables requested.

...
Optional additional arguments to pass on to read.csv of orig data.

Value

A list of tibbles with merged version of all output $TABLEs and the input data. Additional columns will be INNONMEM which will be TRUE for rows that were not ignored by NONMEM. For simulation control files there is also DV_OUT which will contain simulated DV values. DV will always be unmodified from the input dataset.

output_table_first will return a tibble with a single run.

See Also

nm_render(), input_data()

Examples

## requires NONMEM to be installed

## Not run:
## exploratory data plot
read_derived_data("DerivedData/data.csv") %>%
ggplot(aes(x = TIME, y = DV)) +
theme_bw() +
geom_point() +
geom_line(aes(group = ID)) +
facet_wrap(~STUDYTXT)

m1 %>%
output_table_first() %>%
ggplot(aes(x = TIME, y = DV)) +
theme_bw() +
geom_point() +
geom_line(aes(group = ID)) +
facet_wrap(~STUDYTXT) +
## additional layer for overlaying IPRED curves
geom_line(aes(y = IPRED, group = ID))
## End(Not run)
overwrite_behaviour

**Description**

**[Stable]**

This is best used via the "overwrite behaviour" RStudio 'Addin'. Sets the strategy for how to handle overwriting of previously executed control files.

**Usage**

```r
code
```

**Arguments**

- **txt**
  Character either "run", "stop", or "skip".

**Value**

- if `txt` is missing, returns `getOption("nm.overwrite_behaviour")`
  - otherwise returns no value and is called for side effects (setting the `nm.overwrite_behaviour` option).

---

parallel_execute

**Generic execute command for parallelised runs**

**Description**

**[Stable]**

Character to be used with the `cmd()` function to launch a parallelised run.

**Usage**

```r
code
```

**Format**

An object of class character of length 1.

**Details**

Requires cores and parafile fields to be set.
Value

A character object.

See Also

nm_getsetters().

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv")) %>%
    cmd(parallel_execute) %>%
    parafile("/opt/NONMEM/nm75/run/mpilinux8.pnm") %>%
    cores(8)

    cmd(m1)

m2 <- m1 %>% child("m2") ## inherits same command as above

parallel_execute ## view the character to see how psn interfaces with SGE

param_cov_diag  Plot relationship between a parameter and covariate

Description

[Stable]

Plots posthoc parameter-covariate relationships from NONMEM run.

Usage

param_cov_diag(r, param, cov, ..., categorical = FALSE, plot_tv = TRUE)

Arguments

r An nm object.

param Character. Name of parameter.

cov Character. Name of covariate.

... Additional arguments passed to dplyr::mutate().

categorical Logical (default = FALSE).

plot_tv Logical.
**Details**

The `mutate` statement is to add variables not included in original $TABLE.

**Value**

A `ggplot2` plot object.

---

**parent_run**  
*Get parent object of nm object*

---

**Description**

[Stable]

Will pull the parent run of an nm object from the run cache. Run needs to have been executed for this to work.

**Usage**

```r
parent_run(m, n = 1L)
```

**Arguments**

- `m`  
  An nm object.
- `n`  
  Numeric. Generation of parent (default = 1).

**Value**

An nm object. Will not return parent object, if the parent object has not been run.

---

**plot_iter**  
*Plot iterations vs parameters/OBJ*

---

**Description**

[Stable]

Non interactive `ggplot2` based version of the OFV/parameter vs iteration plot in shiny run monitor `shiny_nm()`. Used mainly for inclusion in diagnostic reports.

**Usage**

```r
plot_iter(r, trans = TRUE, skip = 0, yvar = "OBJ")
```
Arguments

r An nm object.

trans Logical (default = TRUE). Should parameter transformations be performed in accordance with $THETA/$OMEGA/$SIGMA comments

skip Numeric (default = 0). The number of iterations to skip when plotting. For observing stationarity it is often useful to remove the beginning iterations where the OFV and parameters may move a lot.

yvar Character (default = "OBJ"). Name of variable/parameter to display.

Value

A ggplot2 object.

See Also

shiny_nm(), nm_render()

Description

[Stable]

Usage

ppc_data(r, FUN, ...,
  pre_proc = identity,
  max_mod_no = NA,
  DV = "DV",
  statistic = "statistic"
)

ppc_whisker_plot(d, group, var1, var2, statistic = "statistic")

ppc_histogram_plot(d, var1, var2, statistic = "statistic")

Arguments

r An nm object (a simulation run).

FUN Statistic function accepting a NONMEM dataset data.frame as an argument and returns data.frame with a column "statistic".
Additional arguments for FUN.

*pre_proc* Function to apply to dataset prior to compute statistics.

*max_mod_no* Integer. Maximum model number to read (set low for debugging).

*DV* Character (default = "DV").

*statistic* Character (default = "statistic"). Name of statistic column returned by FUN.

*d* Output from `ppc_data()`.

*group, var1, var2* Grouping variables for plotting.

### Value

The function `ppc_data()` return a data.frame with observed and predicted statistics. The `ppc_*_plot()` plotting functions return ggplot objects.

### See Also

`nm_render()`

### Examples

```r
## requires NONMEM to be installed
## Not run:

idEXPstat <- function(d, ...) {  # example individual statistic function
  d %>%
    group_by(ID, ...) %>%
    filter(is.na(AMT)) %>%
    summarise(
      AUC = AUC(time = TIME, conc = DV),
      CMAX = max(DV, na.rm = TRUE),
      TMAX = TIME[which.max(DV)]
    ) %>%
    tidyr::gather(key = "exposure", value = "statistic", AUC:TMAX)
  }

EXPstat <- function(d, ...) {  # example summary statistic function
  d %>%
    group_by(exposure, ...) %>%
    summarise(
      median = median(statistic, na.rm = TRUE),
      cv = 100 * sd(statistic, na.rm = TRUE) / mean(statistic, na.rm = TRUE)
    )
}
```

---

**ppc_data**

... Additional arguments for FUN.

*pre_proc* Function to apply to dataset prior to compute statistics.

*max_mod_no* Integer. Maximum model number to read (set low for debugging).

*DV* Character (default = "DV").

*statistic* Character (default = "statistic"). Name of statistic column returned by FUN.

*d* Output from `ppc_data()`.

*group, var1, var2* Grouping variables for plotting.

### Value

The function `ppc_data()` return a data.frame with observed and predicted statistics. The `ppc_*_plot()` plotting functions return ggplot objects.

### See Also

`nm_render()`

### Examples

```r
## requires NONMEM to be installed
## Not run:

idEXPstat <- function(d, ...) {  # example individual statistic function
  d %>%
    group_by(ID, ...) %>%
    filter(is.na(AMT)) %>%
    summarise(
      AUC = AUC(time = TIME, conc = DV),
      CMAX = max(DV, na.rm = TRUE),
      TMAX = TIME[which.max(DV)]
    ) %>%
    tidyr::gather(key = "exposure", value = "statistic", AUC:TMAX)
  }

EXPstat <- function(d, ...) {  # example summary statistic function
  d %>%
    group_by(exposure, ...) %>%
    summarise(
      median = median(statistic, na.rm = TRUE),
      cv = 100 * sd(statistic, na.rm = TRUE) / mean(statistic, na.rm = TRUE)
    )
}
```
tidyr::gather(key = "type", value = "statistic", median:cv)
}
dppc <- m1s %>% ppc_data(EXPstat)
dppc %>% ppc_whisker_plot()
dppc %>% ppc_forest_plot()
## End(Not run)

---

**psn_style_scm**  
*PsN style stepwise covariate method*

**Description**

[Experimental]  
Intent is not to replicate PsN SCM. This is mainly here for illustrative and comparison purposes. Should replicate the model selection in PsN’s SCM functionality with greedy setting.

**Usage**

```r
psn_style_scm(base, run_in, dtest, alpha_forward = 0.05, alpha_backward = 0.01)
```

**Arguments**

- `base`  
  An nm object (base model).
- `run_in`  
  A directory to run in.
- `dtest`  
  Output of `test_relations()`.
- `alpha_forward`  
  Numeric (default = 0.05). Alpha level for forward inclusion.
- `alpha_backward`  
  Numeric (default = 0.01). Alpha level for backward deletion.

**Value**

The nm object of the selected model.

**See Also**

- `test_relations()`, `covariate_step_tibble()`, `bind_covariate_results()`.
**Description**

[Stable]

Read the derived data directly instead of via the nm object which is what `input_data()` does.

**Usage**

```r
read_derived_data(name, na = ".", silent = FALSE, ...)
```

**Arguments**

- **name**: Name or path of file (with or without extension).
- **na**: Character to be passed to `utils::read.csv()`.
- **silent**: Logical (default = `TRUE`). Should messages be suppressed.
- **...**: Additional arguments to be passed to `utils::read.csv()`.

**Value**

A `data.frame` object of the NONMEM dataset.

**See Also**

`write_derived_data()`, `input_data()`, `exclude_rows()`.

**Examples**

```r
## requires NMproject directory structure to operate in
## Not run:
## read a dataset that's been copied into SourceData
d <- read.csv("SourceData/orig_data.csv")
## modify it
d <- d[d$ID < 10, ]
d %>% write DerivedData/data.csv"
## load it again either with
d <- read_derived_data("data")
## or more commonly if it is associated with run (e.g. m1),
## you can use input_data() to load it via the nm object
d <- input_data(m1)
```
remove_parameter

Remove parameter from NONMEM control file

Description

[Stable]
Attempts to remove a parameter from the NONMEM control assuming it has been written according to NMproject conventions (i.e. TVPARAM notation and TVPARAM + IIV_PARAM comments in $\Theta$/OMEGA). The presence of any code that depends on the removed parameter will cause the control file to break.

Usage

remove_parameter(m, name)

Arguments

- m: An nm object.
- name: Character. Parameter name to remove.

Value

An nm object with modified ctl_contents field.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
            based_on = file.path(exdir, "Models", "ADVAN2.mod"),
            data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 <- m1 %>% remove_parameter("KA")
nm_diff(m1)
rename_parameter

Rename a parameter in NONMEM control stream

Description

[Stable]

Usage

rename_parameter(m, ...)

Arguments

m
An nm object.

... Named arguments with character values indicated old names.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 <- m1 %>% rename_parameter(V2 = "V")

m1 %>% dollar("PK")

m1 %>% dollar("THETA")

rmd_to_vignettes

Convert R markdown scripts to vignettes

Description

[Experimental]

Copies (by default) all scripts s01_XXX.Rmd, s02_XXX.Rmd into the "vignettes" and reformats so they meet vignette standards. Use of devtools::build_vignettes() can then be used to build vignettes.

Usage

rmd_to_vignettes(script_files, overwrite = FALSE)
Arguments

script_files  Optional character vector of scripts. If empty will find scripting making the s##_XXX.Rmd convention. Must be .Rmd files
overwrite  Logical (default = FALSE). Overwrites existing vignettes of the same name.

Details

Uses of decision() must pass without stopping so these must have been run interactively prior to use of devtools::build_vignettes().

Value

No return value, called for side effects.

---

Description

[Stable]
Displays the transformed parameters of a completed or running model. Normally used inside of a diagnostic template, but can be useful for quickly seeing parameter estimates of several models.

Usage

rr(m, trans = TRUE)

Arguments

m  An nm object.
trans  Logical. If TRUE (default) will transform using control file $THETA/OMEGA conventions.

Value

A tibble with NONMEM run results.

NONMEM coding conventions used by NMproject

The convention for $THETA comments used by NMproject is value ; name ; unit ; transformation e.g. $THETA 0.1 ; KA ; h-1 ; LOG
The options for THETA transformations are: LOG, LOGIT, RATIO and missing. LOG and LOGIT refer to log and logit transformed THETAs, respectively where the parameters should be back-transformed for reporting. RATIO refers to ratio data types, i.e. parameters that are positive and have a meaningful zero. Most parameters like KA, CL, EMAX fall into this category, but covariates effects which can go negative do not. RSEs are calculated for ratio data. Missing transformations
are suitable for all other parameters, here no RSEs will be calculated, only raw SE values will be reported.

The convention for OMEGA is similar but without a unit item: value ; name ; transformation
e.g. $OMEGA 0.1 ; IIV_KA ; LOG

The options for OMEGA are either LOG or missing. LOG indicating that the individual parameter distribution is log normally distributions and should be reported as a CV% (and associated RSE%) rather than as the raw NONMEM estimate.

The convention for OMEGA is just : value ; name.

**THETA transformations using** trans = TRUE

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\theta$ and se($\theta$) are the NONMEM reported values of parameters and standard errors, respectively:

- **LOG** $FINAL = \exp(\theta)$, $RSE = 100\sqrt{\exp(se(\theta)^2) - 1}$
- **RATIO** $FINAL = \theta$, $RSE = 100se(\theta)/\theta$
- **LOGIT** $FINAL = 100/(1 + \exp(-\theta))$, $SE = se(\theta)$
- **missing** $FINAL = \theta$, $SE = se(\theta)$

**OMEGA transformations using** trans = TRUE

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\omega^2$ and se($\omega^2$) are the NONMEM reported values of parameters and standard errors, respectively:

- **LOG** $FINAL = 100\sqrt{\exp(\omega^2) - 1}$, $RSE = 100(se(\omega^2)/\omega^2)/2$
- **missing** $FINAL = \omega^2$, $SE = se(\omega^2)$

**SIGMA transformations using** trans = TRUE

The value of FINAL and RSE% (always accompanied with a % symbol in outputs) in the returned tibble is the reported standard error (where applicable) where $\sigma^2$ and se($\sigma^2$) are the NONMEM reported values of parameters and standard errors, respectively. All sigmas are reported as standard deviations.

- **all sigmas** $FINAL = \sqrt{\sigma^2}$, $RSE = 100se(\sigma^2)/\sigma^2$

**See Also**

nm_render()
### run_all_scripts

**Run all project scripts sequentially**

**Examples**

```r
## requires NONMEM to be installed
## Not run:

rr(m1)

## compare m1 and m2

rr(c(m1, m2))

## End(Not run)
```

**Description**

[Stable]

Runs/renders all scripts s01 XXX, s02 XXX in the designated "scripts" directory.

**Usage**

```r
run_all_scripts(index, quiet = FALSE)
```

**Arguments**

- `index` Numeric index for subsetting list of scripts before running.
- `quiet` Argument passed to `rmarkdown::render()`.

**Details**


**Value**

Invisibly returns TRUE if file creation is successful.
**run_dir_path**  
Get path to *run_dir*

---

**Description**  
[Stable]  
The function `run_dir()` gives the directory name, whereas this function gets the (relative) path of `run_dir()`.

**Usage**  

```r
run_dir_path(m)
```

**Arguments**  

- `m`  
  An nm object.

**Value**  
A path to the *run_dir* field of `m`.

**See Also**  

`nm_getsetters()`.

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))
run_dir_path(m1)
```

---

**run_nm**  
Run NONMEM jobs

---

**Description**  
[Stable]  
Run nm objects. Uses `system_nm()` to submit the `cmd()` value of object.
Usage

run_nm(
  m,
  ignore.stdout = TRUE,
  ignore.stderr = TRUE,
  quiet =getOption("quiet_run"),
  intern =getOption("intern"),
  force = FALSE,
  cache_ignore_cmd = FALSE,
  cache_ignore_ctl = FALSE,
  cache_ignore_data = FALSE
)

run_nm_batch(m, threads = 10, ...)

Arguments

m             An nm object.
ignore.stdout Logical (default=TRUE). Parameter passed to system_nm().
ignore.stderr Logical (default=TRUE). Parameter passed to system_nm().
quiet         Logical (default=FALSE). Should system_nm() output be piped to screen?
intern        Logical. intern argument to be passed to system_nm().
force         Logical (default = FALSE). Force run even results unchanged.
cache_ignore_cmd Logical (default = FALSE). Should check cmd field with cache?
cache_ignore_ctl Logical (default = FALSE). Should check control file contents with cache?
cache_ignore_data Logical (default = FALSE). Should check dataset with cache?
threads       Numeric. Number of threads to run concurrently.
...           Additional arguments passed to run_nm().

Details

In grid environment it is recommended to run nm_tran() via the RStudio 'Addin' prior to executing this code.

By default, when highlighting code and evaluating it via an RStudio app, run_nm() will not execute and will just return the nm object.

For vector nm objects of length more than 1, all runs will be launched at the same time. This could overwhelm resources if not in a grid environment. In this case see run_nm_batch() for batched execution of a vector valued nm object.

run_nm_batch is a variant of run_nm() containing a threads argument that will submit run_nm()’s in batches and wait for them to complete. If you need all the runs to complete ensure you use a wait_finish() statement afterwards as R console will only be blocked for until the last batch has been submitted which will be before all runs have completed.
## search_raw

**Value**

m with job_info fields populated.

**See Also**

rm_tran()

**Examples**

```r
## requires NONMEM to be installed
## Not run:
m1 <- new_nm(
  run_id = "m1",
  based_on = "staging/Models/ADVAN2.mod",
  data_path = "DerivedData/data.csv"
) %>%
cmd("execute {ctl_name} -dir={run_dir}") %>%
fill_input() %>%
run_nm()

## End(Not run)
```

### Description

[Stable]

Searches through the list of supplied for matching strings of text. Useful in finding files that you know contain certain text snippets.

### Usage

```r
search_raw(files, text, search_title = TRUE, search_contents = TRUE)
```

### Arguments

- **files**: Vector string of files (either names or paths).
- **text**: String (can be regex) to search for.
- **search_title**: Logical (default=TRUE). Should matching occur in title.
- **search_contents**: Logical (default=TRUE). Should matching occur in file contents.

### Value

A subset of files with contents matching text.
setup_code_completion

See Also

ls_scripts(), ls_code_library(), stage()

Examples

ls_scripts("Scripts") %>% search_raw("AUC") ## finds all scripts containing string "AUC"

## regex match find instances of AUC() function being used
ls_scripts("Scripts") %>% search_raw("AUC\(")

## requires NMproject directory structure to operate in
## Not run:
## bring file(s) into project
ls_scripts("/path/to/other/analysis/scripts/dir") %>%
  search_raw("AUC\(") %>%
  import()

## End(Not run)

setup_code_completion  Set up code completion for NMproject

Description

[Experimental]
Intelligent code completion is an experimental way to type NMproject code. This function modifies/creates r.snippets. Needs to be run interactively. Will ask for user confirmation since snippets are an RStudio config setting

Usage

setup_code_completion(force = FALSE, snippet_path = find_snippet_path())

Arguments

force Logical. The default is FALSE which will require user confirmation before editing r.snippets.

snippet_path Character path to the r.snippets file.

Value

No return value, called for side effects.
setup_nm_demo

**setup_nm_demo**  
*Setup demo in current directory*

---

**Description**

[Stable]

Following through the demo is the fastest way to learn the syntax of NMproject. The default demo is a Theophylline ("theopp") pharmacometric analysis. Scripts will be copied numbered s01_XXX.Rmd, s02_XXX.Rmd in the "Scripts" directory and a dataset into "SourceData". The "staging" area will also be pre-filled with the code library model, "ADVAN2.mod". To practice copying this yourself, see `code_library()` for how the app works.

**Usage**

```r
setup_nm_demo(
  demo_name = "theopp",
  overwrite = FALSE,
  additional_demo_locations = NULL
)
```

**Arguments**

- **demo_name**  
  Character. Name of demo. Default = "theopp". See details to find other demos

- **overwrite**  
  Logical. Default changed to FALSE.

- **additional_demo_locations**  
  Character vector. default = NULL. Locations for demo directories.

**Details**

Available demo_name correspond to directory locations in `system.file("extdata","examples",package = "NMproject")`

**Value**

Invisibly returns a tibble with imported file information.

**See Also**

- `code_library()`
sge_parallel_execute

Generic execute command for SGE grids

Description

[Stable]
Character to be used with the `cmd()` function to launch a parallelised job on SGE.

Usage

dge_parallel_execute

Format

An object of class character of length 1.

Details

Requires `cores` and `parafile` fields to be set.

Value

A character object.

See Also

`nm_getsetters()`.

Examples

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv")) %>%
  cmd(sge_parallel_execute) %>%
  parafile("/opt/NONMEM/nm75/run/mpilinux8.pnm") %>%
  cores(8)

cmd(m1)

m2 <- m1 %>% child("m2") ## inherits same command as above

sge_parallel_execute ## view the character to see how psn interfaces with SGE
```
Description

[Stable]
Interactively monitor NONMEM runs. This interface is intentionally limited to monitoring runs, and does not include the ability to create, modify, launch or post-process runs since actions performed in the shiny app are not traceable/reproducible and not part of the workflow you create when scripting.

Usage

shiny_nm(m, envir = .GlobalEnv)

Arguments

m
Either an nm object, or data.frame or list or environment contain nm_lists.

envir
If missing, the environment to search.

Value

No return value, called for side effects.

Examples

if(interactive()){

  # create example object m1 from package demo files
  exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
  m1 <- new_nm(run_id = "m1",
                based_on = file.path(exdir, "Models", "ADVAN2.mod"),
                data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

  shiny_nm() ## use all objects in global workspace
  shiny_nm(m1) ## only m1

  ## if model objects are inside a tibble
  d <- dplyr::tibble(m = m1)

  shiny_nm(d$m) ## only d$m
  shiny_nm(d) ## all nm_lists in d (data.frame/list/environment)

}

**show_ctl**

*Show an uneditable version of the control file*

**Description**

[Stable]

Opens a read-only version of the NONMEM control file for browsing.

**Usage**

```
show_ctl(r)
```

**Arguments**

- `r` An nm object.

**Value**

No return value, called for side effects.

**See Also**

- `show_out()`.

---

**show_out**

*Show an uneditable version of the lst file*

**Description**

[Stable]

Opens a read-only version of the NONMEM control file for browsing.

**Usage**

```
show_out(r)
```

**Arguments**

- `r` An nm object.

**Value**

No return value, called for side effects.

**See Also**

- `show_ctl()`.
simple_field  

*Interface for getting and setting your own simple fields in nm objects*

---

**Description**

[Stable]

**Usage**

```r
simple_field(m, ...)
```

**Arguments**

- `m`: An nm object.
- `...`: Arguments to get/set fields.

**Value**

If `...` contains an assignment, an nm object with modified field, otherwise returns the field value.

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1", 
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 <- m1 %>% simple_field(stars = 3)
m1 %>% simple_field(stars)
m1 ## see that stars is a field of the nm object.
```

---

stage  

*Stage files in project staging area ready for import*

---

**Description**

[Stable]

Staging is a preliminary step of bringing code from external to the project into the project. The intent is it remains a snapshot of code as it was at the time of importing. This aids in reproducibility because if that external code is changed, the staged code will remain fixed.

In practice, this function will rarely need to be used directly. The easiest way to bring code is via the "code library" RStudio `Addin` shiny app.
Usage

stage(
  files,
  root_dir,
  overwrite = FALSE,
  silent = FALSE,
  find_replace_dir_names = TRUE
)

Arguments

files Character vector. path of files to stage.
root_dir Character path to root directory of files. Staged files relative to staging directory will be same as files to root_dir. If this is not specified, will guess based on presence of nm_default_dirs
overwrite Logical (default = FALSE).
silent Logical (default = FALSE).
find_replace_dir_names Logical (default = TRUE). Will attempt to find replace strings in scripts to reflect nm_default_dirs().

Value

A tibble with staged file information.

See Also
code_library(), import()

Examples

## requires NMproject directory structure
## Not run:

ls_code_library("Models/ADVAN2.mod") %>%
  stage()

## End(Not run)
**status**

*Get status of NONMEM runs*

---

**Description**

[Stable]

**Usage**

`status(x)`

**Arguments**

- `x` An `nm` object.

**Value**

A character with the status of the run with values "non started", "running", "finished", or "error"

**See Also**

`status_table()`.

**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1", 
  based_on = file.path(exdir, "Models", "ADVAN2.mod"), 
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

status(m1)  ## not run
```

---

**status_table**

*Get status of multiple runs in form of table*

---

**Description**

[Stable]

A more friendly version of `status()` for vector valued `nm` objects. Useful after bootstraps, or stepwise covariate method steps, or any situation dealing with groups of NONMEM runs.
Usage

status_table(m)

Arguments

m
An nm object.

Value

A tibble object.

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1", 
  based_on = file.path(exdir, "Models", "ADVAN2.mod"), 
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

c(m1, m1) %>% status_table() ## both not started

---

subroutine Subroutine

Description

[Experimental]

Makes the necessary code changes to go from one ADVAN (and TRANS) to another.

Usage

subroutine(m, advan = NA, trans = 1, recursive = TRUE)

Arguments

m
An nm object.

advan
Character. desired ADVAN.

trans
Character. desired TRANS.

recursive
Logical (default = TRUE). Internal argument, do not modify.

Details

Can only switch between subroutines listed in available_advans.

Value

An nm object with modified ctl_contents field.
See Also

advan()

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
            based_on = file.path(exdir, "Models", "ADVAN2.mod"),
            data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

advan(m1) ## 2
trans(m1) ## 1

m1 <- m1 %>% subroutine(advan = 2, trans = 2)

ds <- .available_advans %>%
dplyr::filter(oral) %>%
dplyr::mutate(
    m = m1 %>% child(run_id = label) %>%
      subroutine(advan = advan, trans = trans)
)

ds
ds$m %>% dollar("PK")

---

system_cmd

System/shell command wrapper

Description

[Stable]

Will run getOption("system_cmd"). A OS agnostic interface to the system terminal. Most of the time this will be the same as system_nm except when the PsN/NONMEM execution server is location in a different location to the RStudio server.

Usage

system_cmd(cmd, dir = ".", ...)

Arguments

  cmd  Character. Command to send to shell.
  dir  Optional character. Directory to run command in (default = current working directory)
  ...  Other arguments passed to system command.
Value

The return value of `getOption("system_cmd")`.

Examples

```r
system_cmd("pwd")
```

---

**system_nm**

*System command for NONMEM execution*

Description

[Stable]

Not intended to be used directly in most cases. This is the function used by `run_nm()`. It can also be used directly to launch other PsN commands like `sumo`.

Usage

```r
system_nm(cmd, dir = nm_dir("models"), ...)```

Arguments

- **cmd** Character. System call to be sent to the terminal.
- **dir** Character. Directory (relative path) to run command in. By default this will be the "models" directory (`nm_dir("models")`).
- **...** Additional arguments to be passed to `system()` or `shell()`.

Value

The return value of `getOption("system_nm")`.

See Also

`run_nm()`

Examples

```r
system_nm("hostname")
```

## requires NONMEM to be installed

```r
system_nm("psn --versions")
```

```r
system_nm("sumo run1.mod")
```
system_nm_intern

## End(Not run)

system_nm_intern  Convenience function for system_nm

Description

Used for diagnostic purposes and a backend script for

Usage

system_nm_intern(..., intern = TRUE, ignore.stderr = TRUE, wait = TRUE)

Arguments

...  Arguments passed to system_nm()
intern  Arguments passed to system_nm()
ignore.stderr  Arguments passed to system_nm()
wait  Arguments passed to system_nm()

temp_files  Remove temporary NONMEM files

Description

[Stable]

NONMEM produces a lot of temporary files which can add up to a lot of disk space. One strategy to remove this is to use the clean option in the PsN command. However, this can automatically remove files as soon as the run finishes that may be useful for debugging. ls_tempfiles() allows you to list the paths of all temporary files, for a single run or for all runs for inspection and deletion. clean_tempfiles() is a wrapper function that runs ls_tempfiles() and deletes everything returned. For safety is limited to only deleting files associated with nm objects though.

Usage

ls_tempfiles(
  object = ".",  
  output_loc = c("run_dir", "base"),  
  run_files = NA_character_,  
  include_slurm_files = TRUE,  
  ctl_extension = "mod",  
  include_psn_exports = FALSE
)
clean_run(m, output_loc = c("run_dir", "base"), include_slurm_files = TRUE)

clean_tempfiles(
  object = ".",
  output_loc = c("run_dir", "base"),
  include_slurm_files = TRUE
)

Arguments

object Either an nm object or path to project (default = "."). If a path is specified, the
function will look for all runs in the directory (including subdirectories).

output_loc Optional character for locating files. Either "run_dir" (default) for PsN execu-
tion or "base" for "nmfe" execution.

run_files Optional character vector. Search amongst only these files instead. Default value
NA searches based on object.

include_slurm_files Logical (default = TRUE). Include files generated by Slurm.

ctl_extension Character. Extension of control file (default = "mod")

include_psn_exports Logical (default = FALSE). Considers files that PsN exports to the run_in direc-
tory as temporary

m An nm object

Details

Setting include_psn_exports = TRUE will break 'Pirana' and 'xpose' capability as these software
use exported files.

Value

A character vector of temporary file paths

Examples

# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
  based_on = file.path(exdir, "Models", "ADVAN2.mod"),
  data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

ls_tempfiles(m1) ## if no files, will be empty

m1 %>%
  ls_tempfiles() %>%
  unlink() ## delete all m1 temp files
test_relations

### above line is equivalent to:
clean_tempfiles(m1)

ls_tempfiles() ## display all temp files in analysis project

ls_tempfiles() %>% unlink() ## remove all temp files in analysis project

---

**test_relations**

*Generate tibble of covariate relations to test*

---

**Description**

**[Stable]**

The goal of NMproject’s covariate modelling functions is to provide a stepwise covariate method with manual decision making. This is important to ensure that the full model selection/evaluation criteria (should be defined in statistical analysis plans) can be applied at every step rather than just log likelihood ratio testing, where the most significant model may be unstable, may worsen model predictions or may only be slightly more significant than a more physiologically plausible covariate relationship.

The functions `test_relations()`, `covariate_step_tibble()`, `bind_covariate_results()` together comprise NMproject stepwise covariate method with manual decision. The goal is to be part way between PsN’s SCM and completely manual process at each forward and backward elimination step. The syntax of how covariates are included is the same as PsN’s SCM routine - See PsN documentation for more information.

**Usage**

test_relations(dtest, param, cov, state, continuous)

**Arguments**

- **dtest**: Optional existing `dtest` to append (from an previous use `test_relations()`).
- **param**: Character. Name of parameter(s).
- **cov**: Character. Name of covariate(s).
- **state**: Numeric or character. Number/name of state (see details).
- **continuous**: Logical (default = TRUE). If FALSE, will treat the covariate as categorical.

**Details**

Setting vector values for param, cov, and state, will expand the grid to test each value with every other value greedily. This is similar to `expand.grid()` available states (see also `add_cov()`):

- "2" or "linear"  PARCOV=( 1 + THETA(1)*(COV -median))
- "3" or "hockey-stick"  IF(COV.LE.median) PARCOV = ( 1 + THETA(1)*(COV - median)) IF(COV.GT.median) PARCOV = ( 1 + THETA(2)*(COV - median))
"4" or "exponential"  \( \text{PARCOV} = \exp(\theta_1 \times (\text{COV} - \text{median})) \)

"5" or "power"  \( \text{PARCOV} = ((\text{COV}/\text{median})^{\theta_1}) \)

"power1"  \( \text{PARCOV} = ((\text{COV}/\text{median})^{1}) \)

"power0.75"  \( \text{PARCOV} = ((\text{COV}/\text{median})^{0.75}) \)

"6" or "log-linear"  \( \text{PARCOV} = (1 + \theta_1 \times (\log(\text{COV}) - \log(\text{median}))) \)

**Value**

A tibble describing relationships to test.

**See Also**

`add_cov()`, `covariate_step_tibble()`, `bind_covariate_results()`

**Examples**

```r

dtest <- test_relations(param = c("KA", "K", "V"),
                        cov = c("LIN1", "LIN2", "LIN3", "RND1", "RND2", "RND3"),
                        state = c("linear", "power"),
                        continuous = TRUE) %>%
  test_relations(param = c("KA", "K", "V"),
                cov = "BN1",
                state = "linear",
                continuous = FALSE)

dtest
```

**update_parameters**  
Update initial estimates to final estimates

**Description**

[Stable]

**Usage**

`update_parameters(ctl, from)`

**Arguments**

- `ctl`  
  An nm object.

- `from`  
  Optional nm object. The completed object from which to extract results. If not specified, `from` will be taken to be `ctl`.

**Value**

An nm object with modified `ctl_contents` field.
Examples

```
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
              based_on = file.path(exdir, "Models", "ADVAN2.mod"),
              data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>% dollar("THETA")

## requires NONMEM to be installed
## Not run:

m1 %>% run_nm() %>% wait_finish()
m1 <- m1 %>% update_parameters()
m1 %>% dollar("THETA")

## End(Not run)
```

wait_finish

**Wait for runs to finish**

**Description**

[Stable]

Blocks subsequent R execution until run(s) are finished. This is useful for when subsequent relies on outputs from completed NONMEM jobs. It is normally a good idea to include this in post processing R markdown templates, to ensure they wait for runs to complete before executing.

**Usage**

```
wait_finish(r, timeout = NA)
```

**Arguments**

- `r` An nm object.
- `timeout` Numeric seconds to wait before timeout.

**Value**

Invisibly returns `r` unmodified. Called for side effects.

**Examples**

```
## requires NONMEM to be installed

## Not run:
```
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
    based_on = file.path(exdir, "Models", "ADVAN2.mod"),
    data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

m1 %>%
  run_nm() %>%
  wait_finish()

## following requires run to be completed.
covariance_plot(m1)

## End(Not run)

---

wait_for

### Wait for statement to be TRUE

**Description**

[Stable]

Will block R console until an expression evaluates to be TRUE.

**Usage**

```r
wait_for(x, timeout = NULL, interval = 1)
```

**Arguments**

- `x` Boolean expression to evaluate.
- `timeout` Numeric. Maximum time (in seconds) to wait.
- `interval` Numeric. Number of seconds (default=1) to wait before rechecking.

**Value**

Invisibly returns TRUE indicating value of `x` after waiting for `x` to be TRUE.

**See Also**

`wait_finish()`.
**Examples**

```r
# create example object m1 from package demo files
exdir <- system.file("extdata", "examples", "theopp", package = "NMproject")
m1 <- new_nm(run_id = "m1",
             based_on = file.path(exdir, "Models", "ADVAN2.mod"),
             data_path = file.path(exdir, "SourceData", "THEOPP.csv"))

## requires NONMEM to be installed
## Not run:
## the following are identical
m1 %>% run_nm() %>% wait_finish()

wait_for(is_finished(m1)) ## wait_finish is a more convenient form of this

## End(Not run)
```

---

**wipe_run**

*Wipe previous run files*

**Description**

[Stable]

Will remove all the output files generated by a previously completed run. This is run by `run_nm()` prior to launching any jobs to ensure that output files from old runs do not get mistaken for up-to-date runs.

**Usage**

```r
wipe_run(r)
```

**Arguments**

- `r`  
  An nm object.

**Value**

No return value, called for side effects.
write_derived_data  Write derived data file

Description

[Stable]

Will write a dataset and an .RDS version of it to the (by default) "DerivedData" directory. The main benefit of the .RDS dataset is that functions like `input_data()` and `output_table()` can use it for rapid reading speeding up overall function.

Usage

```r
write_derived_data(d, name, ...)
```

Arguments

- `d`: A data.frame. Data frame to be saved.
- `name`: Character. Name of file (with or without extension). If not a path, will save to DerivedData directory.
- `...`: Additional arguments to be passed to `utils::write.csv()`.

Details

If there is no "DerivedData" data directory and you are using a different structure the argument `name` must be a (relative) path to an existing directory where you want your NONMEM ready dataset to be stored.

Value

No return value, called for side effects.

See Also

`read_derived_data()`, `input_data()`, `exclude_rows()`

Examples

```r
## requires NMproject directory structure to operate in
## Not run:
## read a dataset that's been copie into SourceData
d <- read.csv("SourceData/orig_data.csv")

## modify it
d <- d[d$ID < 10, ]

d %>% write_derived_data("DerivedData/data.csv")
```
## load it again either with

\[d \leftarrow \text{read\_derived\_data\("data\")}\]

## or more commonly if it is associated with run (e.g. m1),
## you can use input\_data() to load it via the nm object

\[d \leftarrow \text{input\_data(m1)}\]

## End(Not run)

---

Function pipe for nm objects

**Description**

**[Experimental]**

Pipe an nm object object to a list of functions. Although this enables multiple NONMEM runs to be handled simultaneously, it does make your code less readable.

**Usage**

\[lhs \%f\% rhs\]

**Arguments**

- **lhs** An nm object.
- **rhs** A list of functions. Must be same length as lhs.

**Value**

A modified nm object.

**See Also**

- `child()` for creating multiple child NONMEM objects

**Examples**

# create example object m1 from package demo files

\[\text{exdir} \leftarrow \text{system\_file\("extdata", "examples", "theopp", package = "NMproject")}\]

\[\text{m1} \leftarrow \text{new\_nm(run\_id = "m1",}\]

\[
\text{based\_on = file\_path(exdir, "Models", "ADVAN2.mod"),}\]

\[
\text{data\_path = file\_path(exdir, "SourceData", "THEOPP.csv")}\]

\[\text{temp\_data\_file} \leftarrow \text{paste0(tempfile(), ".csv")}\]

## dataset has missing WTs so create a new one and assign this to the run
input_data(m1) %>%
  dplyr::group_by(ID) %>%
  dplyr::mutate(WT = na.omit(WT)) %>%
  write_derived_data(temp_data_file)

m1 <- m1 %>% data_path(temp_data_file)

mWT <- m1 %>% child(c("m2", "m3", "m4")) %>%
      list(
        . %>% add_cov(param = "V", cov = "WT", state = "linear"),
        . %>% add_cov(param = "V", cov = "WT", state = "power"),
        . %>% add_cov(param = "V", cov = "WT", state = "power1")
      )

mWT %>% dollar("PK")

unlink(temp_data_file)
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