EXECUTE user guide

2013-05-28 PsN 3.6.2

Introduction

The execute script is a PsN tool allows you to run multiple modelfiles either sequentially or in parallel. It is an nmfe replacement with advanced extra functionality.

Execute creates subdirectories where it puts NONMEMs input and output files, to make sure that parallel NONMEM runs do not interfere with each other. The top directory is by default named 'modelfit_dirX' where 'X' is a number that starts at 1 and is increased by one each time you run execute.

Example
execute -threads=2 -retries=5 phenobarbital.mod pheno_alternate.mod

The parallel_retries script

The retries (see documentation in common_options_defaults_versions_psn.pdf) are always done serially in execute and other PsN programs. The parallel_retries script is a help script that takes a single model as input, creates 'min_retries' extra copies of this model with tweaked initial estimates, and then runs the original plus the extra models in parallel in separate NM_run subdirectories. Results are summarized in raw_results.csv in the run directory. The script does not select the best retry, but the user must do that manually based on raw_results.csv. The script parallel_retries takes the same input as execute, except that only a single model is accepted as input, and option -min_retries is required.

Example:
parallel_retries run33.mod -min_retries=4 -threads=5 -seed=12345

Input and options

Required execute input

A model file is required on the command-line.

Optional input

All options listed in common_options_defaults_versions_psn.pdf apply to execute and parallel_retries. Those are the most important options for execute. They were originally implemented for this tool, but now they are common to most PsN scripts.

In addition, unique to execute and parallel_retries:

-model_dir_name	Default not used. This option changes the basename of the run directory from modelfit_dir to <modelfile>.dir. where <modelfile> is the name of the first model file in the list given as arguments to execute. The directories will be numbered starting from 1, increasing the number each time execute

	is run with a model file with the same name. If the option directory is used it will override -model_dir_name.
-prepend_options_to_lst	Default not used. This option makes PsN prepend the final lst-file (which is copied back to the directory from which execute was called) with the file version_and_option_info.txt which contains run information, including all actual values of optional PsN options. PsN can still parse the lst-file with the options prepended, so the file can still be used it as input to e.g. sumo, vpc or update_inits. Disabled with -no-prepend_options_to_lst if set in psn.conf.
-tail_output	Default not used. This option only works for execute under Windows. Option -tail_output specifies that execute should invoke a program (tail) that displays the output file, including the gradients, during minmization. The tail program is started automatically but it is up to the user to terminate the program. For the tail_output option to work, a third party tail program must be installed. Tail programs that are known to work are WinTail and Tail for Win32. The latter is recommended and can be downloaded at http://tailforwin32.sourceforge.net. It is also necessary to have correct settings of the variables wintail_exe, which is the path to the tail program, and wintail_command, which is the command for the tail program. The defaults, which work for the Tail for Win32 package, are seen below. These two variables can be set to other values in psn.conf.
-wintail_exe='string'	Default “C:\\Program Files\\Tail-4.2.12\\Tail.exe”. Only for Windows. See tail_output for description.
-wintail_command='string'	Default "tail OUTPUT”. Only for Windows. See -tail_output for description.
-copy_data	Default set. Disable with -no-copy_data. By default, PsN will copy the datafile into NM_run1 and set a local path in psn.mod, the actual modelfile run with NONMEM. If -no-copy_data is set, PsN will not copy the data to NM_run1 and instead set a global path to the datafile in psn.mod.

Output

When the NONMEM runs are finished, the output and table files will be copied to the directory where execute started in which means that you can normaly ignore the 'modelfit_dirX' directory. If you need to access any special files you can find them inside the 'modelfit_dirX'. Inside the 'modelfit_dirX' you find a few subdirectories named 'NM_runY'. For each model file you specified on the command line there will be one 'NM_runY' directory in which the actual NONMEM execution takes place. The order of the 'NM_runY' directories corresponds to the order of the modelfiles given on the command line. The first run will take place inside 'NM_run1', the second in 'NM_run2' and so on.