GLS userguide

2013-05-28 PsN 3.6.2

Overview

During the modelling process one may encounter scenarios where first-order conditional estimation with ε-η interaction (FOCEI) is indicated but may be prohibitively time consuming or unstable. Also, it may be a concern that a misspecification of the residual error model may translate to bias in structural or inter-individual variability parameters. These two problems may be overcome by using a generalised least squares (GLS) type approach where dependent variable predictions are obtained from a previous model fit and then used in the residual error model. The gls program automates this procedure.

In summary the GLS method amounts to the following: Run the original model. In a second step IPRED is replaced with GLSP in the definition of W where GLSP is computed as

$PRED_{orig} \cdot iwres\_shrinkage + (1-iwres\_shrinkage_{orig})*IPRED_{orig}$,

where $PRED_{orig}$ and $IPRED_{orig}$ are obtained from running the original model and iwres_shrinkage is either a population shrinkage obtained from the original model run or a per-observation shrinkage based on simulations. The modified gls model is then estimated.

Example

gls run1.mod

Input and options

Required input

A model file is required on the command-line.

Optional input

-ind_shrinkage	Default not set. Compute per-observation iwres-shrinkage based on simulations.
-samples=N	Default not used. Only relevant if -ind_shrinkage is set and -gls_model is not set. Creates N copies of input model with different seeds in \$SIM. Run to get N IWRES values for each data point y_{ij}. Compute $iwres\_shrinkage_{ij} = 1-stdev(IWRES_{ij}(1:N))$
-reminimize	Default not set. Only relevant if -ind_shrinkage is set and -gls_model is not set. By default, simulated datasets will be run with MAXEVAL=0 (or equivalent for non-classical estimation methods). If option -reminimize is set then the same \$EST as in the input model will be used.
-additive_theta=XX	Default not used. In gls model, add a small and fix additive error in W. The error is added by changing W=SQRT(<expression>) to W=SQRT(THETA(T)**2+<expression>) in the gls model, where T is the order number of new \$THETA XX FIX added to the model.

-iwres_shrinkage=X	Default not used. Forbidden in combination with -ind_shrinkage. If the population iwres shrinkage from the input model run is already available, or if a special values such as 0 or 1 is desired, the user can give the value as input on the command-line. Important note: PsN reports shrinkage in percent in the raw_results file, so if using the value from raw_results as input that value must be divided by 100.
-gls_model	Default not set. Only possible together with option -iwres_shrinkage or -ind-shrinkage. This option is to be used when a datafile with all data needed for the gls model run is already available, i.e. all input for the original model plus columns with PRED and IPRED from the original model run, and if -ind_shrinkage is set also a ISHR column with per observation shrinkage values. The option indicates that $DATA specifies the file with the gls input data, and that $INPUT lists the parameters in the datafile. In $INPUT the columns PPRE and PIPR must be present as headers for PRED and IPRED values, plus ISHR for the shrinkage column if -ind_shrinkage is set.
	Then PsN will add the GLSP code to the gls model and run it directly, saving the original model run.
	Note that a run with the ebe_npde program will automatically generate a complete input file for gls (including PRED IPRED and per-observation shrinkage).
-sim_table	Default not set. Only relevant if -ind_shrinkage is set and -gls_model is not set. PsN will delete all existing $TABLE in the simulation models before adding a $TABLE for per-observation IWRES values, but if option -sim_table is set then an extra $TABLE with diagnostic output is added to each simulation model.
-set_simest	Default not set. Only relevant if -gls_model is not set. This option can be used to set different $EST for original, simulation (if used) and final gls models, and to set a custom $SIM for the simulation model. When this option is set, PsN will look for lines starting with certain tags in the input model. All lines starting with the tag
	;gls-final
	will be collected, the tag will be removed, and then PsN will check that the lines define a single $EST record. This $EST record will be set in the final model, instead of the one in the input model. If no ;gls-final tag is found the $EST record in the final model will be the same as in the input model. All lines starting with the tag
	;gls-sim
	will also be collected, the tag will be removed, and then PsN will check that the lines define either a single $EST or a single $SIM, or one of each. If a $SIM record is defined this will be used in the simulation model instead of any $SIM found in the input model. If a $EST record is defined this will be used in the simulation model instead of the $EST found in the input model.

Some common PsN-options useful with gls

For a complete list of common options see common_options_defaults_versions.pdf, or psn_options -h on the commandline.

-directory=gls_dirN   The run directory can be named.
-help   With -help gls will print a longer help message.

Output

The results are in the raw_results file. If -ind_shrinkage is set the individual shrinkage values are in ind_iwres_shrinkage.dta. All lst-files, model files and table files are in the m1 subdirectory.

Procedure overview

Original input model (only done if -gls_model is not set):

1. If option -additive_theta=XX is set, add $THETA XX FIX as last $THETA. Store order number T of new theta.

2. Remove MSFO option from $EST, if present.

3. If the model has both $PRIOR and $SIM then set option TRUE=PRIOR in $SIM.

4. Remove $COVARIANCE, if present.

5. If a lst-file is found for the input model, update initial estimates in input model based on lst-file.

6. Copy undropped $INPUT variables to new $TABLE. In $TABLE add IPRED PRED. Add NOPRINT ONEHEADER NOAPPEND FILE=glsinput.dta

7. Run modified original input model. Let PsN compute iwres-shrinkage for this model regardless if option -ind_shrinkage or -iwres_shrinkage is set.

Simulation models (only done if option -ind_shrinkage is set and -gls_model is not set):

1. Create 'samples' copies of modified original input model after modifications step 1-4 above.

2. If $SIM not present, create simple $SIM (1234 NEW). Seed and NSUB will be set below.

3. If option -set_simest is set and a simulation record behind the tag ;gls-sim is found, use this new simulation record instead.

4. In each copy set unique seed in $SIM and set NSUB=1.

5. Set IGNORE=@ since datafile will get a header during copying. Keep any IGNORE=(...).

6. Unless option reminimize is set, set MAXEVAL=0 (or corresponding for non-classical estimation methods).

7. If option -set_simest is set and an estimation record behind the tag ;gls-sim is found, use this new estimation record instead. Do not change MAXEVAL in this new estimation record.

8. If ONLYSIM is found in $SIM then remove the $EST record.

9. Update initial estimates with output from running modified original input model (step 7 above).

10. Remove existing $TABLE.

11. In each sim model, set $TABLE IWRES ID NOPRINT ONEHEADER NOAPPEND FILE=iwres_<order number>.dta.

12. If option -sim_table is set: In each sim model set an extra $TABLE

with ID TIME IPRED W IWRES NOPRINT ONEHEADER FILE=sdtab-sim<order number>.dta to be used e.g. for diagnostics.

13. Run 'samples' sim models. Let PsN compute iwres-shrinkage for all of them.

14. Read all iwres_<order number>.dta files, storing all IWRES values per data point. Compute, per data point, ISHR_ij=1-stdev(IWRES_ij). Open glsinput.dta and append ISHR column with computed values. Print also shrinkage column to new file ind_iwres_shrinkage.dta

GLS model if option -gls_model is not set:

1. Copy modified original input model after modifications step 1-3 in original input model section.

2. Remove DROP columns completely from $INPUT. Add variables PIPR and PPRE. If -ind_shrinkage is set add variable ISHR.

3. remove $SIM if present

4. If $PRIOR is set, remove option PLEV

5. Update initial estimates with output from running modified original input model.

6. change filename in $DATA to glsinput.dta.

7. If option -set_simest is set and an estimation record is found behind the tag ;gls-final then use this estimation record instead of the old one.

8. If $TABLE is present: append -gls to filename set with FILE to distinguish from table output from original model.

9. Set IGNORE=@ in $DATA. Skip all old IGNOREs (glsinput.dta is filtered).

10. In $DATA add option IGNORE=(PIPR.LE.0.000000001)

11. add code in the very beginning of $PRED/$ERROR

SHRI = <iwres_shrinkage from input model run or iwres_shrinkage option or ISHR if if -ind_shrinkage is set>

IF(SHRI.LE.0) SHRI = 0

GLSP = SHRI*PPRE + (1-SHRI)*PIPR

12. check that W definition is of the form W=SQRT(...IPRED...) and replace IPRED with GLSP in W definition. If option -additive_theta=XX is set, prepend THETA(T)**2+ to the expression inside parentheses of W=SQRT(...) where T is order number of new THETA.

13. Do 12) for every line of the form W=SQRT (...IPRED...).

14. Run gls model. Let PsN compute iwres shrinkage for this model. Append raw_results to raw_results of original model, if original model was run.

GLS model if option -gls_model is set:

1. If option -additive_theta=XX is set, add $THETA XX FIX as last $THETA. Store order number

T of new theta.

2. Remove MSFO option from $EST, if present.

3. If a lst-file is found for the gls model, update initial estimates in gls model based on lst-file.

4. In $DATA add option IGNORE=(PIPR.LE.0.000000001)

5. add code in the very beginning of $PRED/$ERROR

SHRI = <iwres_shrinkage from input model run or iwres_shrinkage option or ISHR if if -ind_shrinkage is set>

IF(SHRI.LE.0) SHRI = 0

GLSP = SHRI*PPRE + (1-SHRI)*PIPR

6. check that W definition is of the form W=SQRT(...IPRED...) and replace IPRED with GLSP in W definition. If option -additive_theta=XX is set, prepend THETA(T)**2+ to the expression inside parentheses of W=SQRT(...) where T is order number of new THETA.

7. Do 6) for every line of the form W=SQRT (...IPRED...).

8. Run gls model. Let PsN compute iwres shrinkage for this model. Append raw_results to raw_results of original model, if original model was run.