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bayesstats grubin — Gelman–Rubin convergence diagnostics

Description Quick start

Quick start Menu Syntax
Remarks and examples Stored results Methods and formulas

References Also see

Description

Options

bayesstats grubin calculates Gelman-Rubin convergence diagnostics for model parameters and functions of model parameters using current Bayesian estimation results containing at least two Markov chains

Quick start

Gelman-Rubin convergence diagnostics for all model parameters after a Bayesian regression model using four chains

```
bayes, nchains(4): regress y x1
bayesstats grubin
```

Same as above, but only for model parameters {y:x1} and {sigma2} bayesstats grubin {y:x1} {sigma2}

Gelman-Rubin convergence diagnostics for functions of scalar model parameters bayesstats grubin ({y:x1}-{y:_cons}) (sd:sqrt({sigma2}))

Menu

Statistics > Bayesian analysis > Gelman-Rubin convergence diagnostics

Syntax

Convergence statistics for all model parameters

```
bayesstats grubin [, options showreffects[(reref)]]
bayesstats grubin _all [, options showreffects[(reref)]]
```

Convergence statistics for selected model parameters

```
bayesstats grubin paramspec [, options]
```

Convergence statistics for functions of model parameters

```
bayesstats grubin exprspec [, options]
```

Full syntax

```
bayesstats grubin spec [spec ...] [, options]
```

paramspec can be one of the following:

{eqname:param} refers to a parameter param with equation name eqname;

{eqname:} refers to all model parameters with equation name eqname;

{eqname:paramlist} refers to parameters with names in paramlist and with equation name eqname; or

{param} refers to all parameters named param from all equations.

In the above, *param* can refer to a matrix name, in which case it will imply all elements of this matrix. See *Different ways of specifying model parameters* in [BAYES] **Bayesian postestimation** for examples.

exprspec is an optionally labeled expression of model parameters specified in parentheses:

```
([exprlabel:]expr)
```

exprlabel is a valid Stata name, and expr is a scalar expression that may not contain matrix model parameters. See Specifying functions of model parameters in [BAYES] Bayesian postestimation for examples.

spec is one of paramspec or exprspec.

options	Description
sort	list parameters in descending order of their convergence statistics
skip(#)	skip every # observations from the MCMC sample; default is skip(0)
nolegend display_options	suppress table legend control spacing, line width, and base and empty cells

collect is allowed; see [U] 11.1.10 Prefix commands.

Options

sort specifies that model parameters be listed in descending order of their Gelman-Rubin convergence statistics. This option is useful for models with many parameters, such as multilevel models, to more easily identify the set of parameters with large values of convergence statistics.

showreffects and showreffects(*reref*) are for use after multilevel models, and they specify that the results for all or a list *reref* of random-effects parameters be provided in addition to other model parameters. By default, all random-effects parameters are excluded from the results to conserve computation time. If random-effects parameters are of interest in your study, you should use option showreffects to check their convergence diagnostics.

skip(#) specifies that every # observations from the MCMC sample not be used for computation. The default is skip(0) or to use all observations in the MCMC sample. Option skip() can be used to subsample or thin the chain. skip(#) is equivalent to a thinning interval of #+1. For example, if you specify skip(1), corresponding to the thinning interval of 2, the command will skip every other observation in the sample and will use only observations 1, 3, 5, and so on in the computation. If you specify skip(2), corresponding to the thinning interval of 3, the command will skip every 2 observations in the sample and will use only observations 1, 4, 7, and so on in the computation. skip() does not thin the chain in the sense of physically removing observations from the sample, as is done by, for example, bayesmh's thinning() option. It only discards selected observations from the computation and leaves the original sample unmodified.

nolegend suppresses the display of the table legend, which identifies the rows of the table with the expressions they represent.

display_options: vsquish, noemptycells, <u>base</u>levels, <u>allbase</u>levels, <u>nofvlab</u>el, fvwrap(#), fvwrapon(style), and nolstretch; see [R] Estimation options.

Remarks and examples

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Remarks are presented under the following headings:

Gelman–Rubin convergence diagnostic Using bayesstats grubin

Gelman-Rubin convergence diagnostic

The Gelman–Rubin convergence diagnostic, R_c , assesses MCMC convergence by analyzing differences between multiple Markov chains. The convergence is assessed by comparing the estimated between-chains and within-chain variances for each model parameter. Large differences between these variances indicate nonconvergence. See Gelman and Rubin (1992) and Brooks and Gelman (1998) for details.

Large values of R_c indicate nonconvergence of MCMC. Literature suggests that the values of this diagnostic should be less than 1.2 for all model parameters to declare MCMC convergence. In practice, a more stringent convergence rule, $R_c < 1.1$, is often used.

Gelman-Rubin diagnostic relies on a Student's t approximation of the marginal posterior distribution of a model parameter. When this assumption is suspect, it is recommended to transform the parameter such that its marginal posterior distribution is better approximated by a Student's t distribution before obtaining the diagnostic. For example, for the variance parameter, it is better to compute the diagnostic for the log variance.

Using bayesstats grubin

The bayesstats grubin command computes the Gelman-Rubin convergence diagnostic for each model parameter using multiple MCMC samples or chains from a common posterior model. This command requires at least two chains. Multiple chains can be obtained by using the nchains() option with the bayesmh command ([BAYES] bayesmh) or with the bayes prefix ([BAYES] bayes). When you simulate multiple chains to assess convergence, it is important to use overdispersed initial values (Gelman and Rubin 1992, Brooks and Gelman 1998). See Specifying initial values in [BAYES] bayesmh and Initial values in [BAYES] bayes for details.

When typed without arguments, the command displays results for all model parameters. Alternatively, you can specify a subset of model parameters following the command name; see *Different ways of specifying model parameters* in [BAYES] **Bayesian postestimation**. You can also obtain results for scalar functions of model parameters; see *Specifying functions of model parameters* in [BAYES] **Bayesian postestimation**. Also see example 2.

For multilevel models, similarly to other Bayesian postestimation commands, bayesstats grubin does not report convergence statistics for the random-effects parameters by default. You can use the showreffects option to see them for all random-effects parameters or the showreffects (*reref*) option for a subset *reref* of random-effects parameters of interest. See *Multilevel models* in [BAYES] bayes for more information about MCMC convergence in multilevel models.

For models with many parameters such as multilevel models, you can use the sort option to list model parameters in descending order of their convergence statistics Rc. The parameters with the largest values of Rc will be listed first, making it easier to verify their convergence.

Example 1: Convergence diagnostics for all parameters

Recall our analysis of womenwage.dta using the bayes: regress command from example 1 in [BAYES] bayes. We fit a linear regression model to the response variable wage with predictor age. Here we use option nchains(3) to simulate three Markov chains to formally check convergence of model parameters. To ensure reproducibility of multiple chains, we also specify the rseed(15) option. Specifying set seed is not sufficient for reproducibility with multiple chains; see *Reproducing results* in [BAYES] bayesmh for details.

```
. use https://www.stata-press.com/data/r18/womenwage
(Wages of women)
. bayes, nchains(3) rseed(15): regress wage age
Chain 1
  Burn-in ...
  Simulation ...
Chain 2
  Burn-in ...
  Simulation ...
Chain 3
  Burn-in ...
  Simulation ...
Model summary
Likelihood:
  wage ~ regress(xb_wage,{sigma2})
Priors:
  {wage:age _cons} ~ normal(0,10000)
                                                                               (1)
          {sigma2} ~ igamma(.01,.01)
(1) Parameters are elements of the linear form xb_wage.
Bayesian linear regression
                                                Number of chains
                                                                                 3
Random-walk Metropolis-Hastings sampling
                                                Per MCMC chain:
                                                                           12,500
                                                    Iterations
                                                                            2,500
                                                    Burn-in
                                                    Sample size
                                                                           10,000
                                                Number of obs
                                                                              488
                                                Avg acceptance rate =
                                                                             .3673
                                                Avg efficiency: min =
                                                                             .1409
                                                                             .1735
                                                                 avg =
                                                                             .2294
                                                                 max =
Avg log marginal-likelihood = -1810.1557
                                                Max Gelman-Rubin Rc =
                                                                 Equal-tailed
                     Mean
                            Std. dev.
                                           MCSE
                                                    Median
                                                             [95% cred. interval]
wage
                 .4003528
                             .0599411
                                        .000922
                                                  .4002037
                                                              .2804134
                                                                          .5188627
         age
                 5.999502
                            1.769855
                                        .026358
                                                  6.025288
                                                              2.571305
                                                                         9.517341
       _cons
                90.80977
                            5.822896
                                        .070195
                                                  90.49567
                                                              79.92114
                                                                         102.7621
      sigma2
```

Note: Default priors are used for model parameters.

Note: Default initial values are used for multiple chains.

Compared with example 1 in [BAYES] **bayes**, the precision of the posterior means almost doubled with more chains, judging by the MCMC standard errors. For example, the MCSE estimate for {sigma2} drops from 0.12 to 0.07.

In the presence of multiple chains, the bayes prefix automatically reports in the header the maximum value of the Gelman–Rubin convergence statistics across all parameters. In practice, we want to see this value be close to 1; if it is less than 1.1, the chains are considered to have converged. This convergence rule is satisfied in our example.

To compute the Gelman-Rubin statistics for all model parameters, we type bayesstats grubin without arguments after the bayes prefix.

. bayesstats grubin

Gelman-Rubin convergence diagnostic

Number of chains = 3

MCMC size, per chain = 10,000

Max Gelman-Rubin Rc = 1.000323

		Rc
wage	age _cons	1.000062 1.000323
	sigma2	1.000253

Convergence rule: Rc < 1.1

Just like the bayes prefix, the bayesstats grubin command reports in the header the maximum value of Rc across all parameters. This is particularly useful as a quick convergence check for models with many parameters: if the maximum Rc is less than 1.2 or 1.1, then this convergence rule is satisfied by all parameters. In our example, the maximum Rc is 1.0003 and is less than 1.1, so the convergence criterion is met for all parameters.

The table reports the Rc estimates for each model parameter. As we already determined based on the maximum Rc, the convergence diagnostics for all model parameters are less than 1.1. This suggests that all chains have converged.

Example 2: Convergence diagnostics for functions of parameters

Continuing with example 1, we can compute the Gelman-Rubin statistics for functions of parameters. Let's compute the convergence diagnostic for the log-transformed variance parameter {sigma2}.

. bayesstats grubin (lnsigma2: ln({sigma2}))

Gelman-Rubin convergence diagnostic

Number of chains = 3

MCMC size, per chain = 10,000

Max Gelman-Rubin Rc = 1.000268

lnsigma2 : ln({sigma2})

	Rc
lnsigma2	1.000268

Convergence rule: Rc < 1.1

Again, the convergence diagnostic for the log-transformed variance is less than 1.1 indicating no convergence problems with the transformed parameter. This also suggests that {sigma2} does not have convergence problems.

In our examples, we used the default initial values provided by bayes: with multiple chains; see *Initial values* in [BAYES] **bayes**. To fully explore MCMC convergence, particularly when a posterior distribution is suspected to have multiple modes, you should use overdispersed initial values. See

4

4

Multiple chains using overdispersed initial values in [BAYES] bayesmh for an example of how to specify overdispersed initial values.

Of course, it is important to explore convergence visually as well; see Convergence diagnostics using multiple chains in [BAYES] bayesmh.

Stored results

bayesstats grubin stores the following in r():

Scalars	
r(mcmcsize) r(nchains) r(Rc_max)	MCMC sample size of each chain number of MCMC chains maximum convergence diagnostic
Matrices	
r(Rc)	convergence diagnostics Rc
$r(t_df)$	degrees of freedom of a t distribution
r(B)	between-chains variances
r(W)	within-chain variances
r(V)	total variances

Methods and formulas

Suppose we have M chains of length T. For a model parameter θ , let $\{\theta_{jt}\}_{t=1}^T$ be the jth simulated chain drawn from the marginal posterior distribution of θ , $j=1,\ldots,M$. Let $\widehat{\theta}_j$ and \widehat{s}_j^2 be the respective sample posterior mean and variance of the mth chain, and let the overall sample posterior mean be $\widehat{\theta} = (1/M) \sum_{j=1}^{M} \widehat{\theta}_{j}$. The between-chains and within-chain variances are given by

$$B = \frac{T}{M-1} \sum_{j=1}^{M} (\widehat{\theta}_j - \widehat{\theta})^2$$

$$W = \frac{1}{M} \sum_{j=1}^{M} \hat{s}_j^2$$

When the chains are strongly stationary, that is, all chains draw samples from the target posterior distribution, the weighted average of W and B

$$\widehat{\sigma}^2 = \frac{T-1}{T}W + \frac{1}{T}B$$

is an unbiased estimator of the marginal posterior variance of θ .

Gelman and Rubin (1992) approximate the target distribution of θ by a Student's t distribution with mean $\widehat{\theta}$ and scale $\sqrt{\widehat{V}}$, where

$$\widehat{V} = \frac{T-1}{T}W + \frac{M+1}{MT}B$$

They define the so-called "scale" reduction factor as the ratio of \hat{V} and $\sigma^2 = \text{Var}(\theta)$. They further estimate σ^2 by W and use the ratio of \hat{V} and W as an estimator of the scale reduction factor, known as the potential scale reduction factor. If the M chains have converged to the target posterior distribution, then the potential scale reduction factor should be close to 1.

Brooks and Gelman (1998) propose the corrected estimator of the potential scale reduction factor, R_c , that accounts for sampling variability:

$$R_c = \sqrt{\frac{\hat{d}+3}{\hat{d}+1}} \frac{\hat{V}}{W}$$

where \widehat{d} is the estimated degrees of freedom of the approximating Student's t distribution for θ

$$\widehat{d} = \frac{2\widehat{V}^2}{\widehat{\operatorname{Var}}(\widehat{V})}$$

and

$$\begin{split} \widehat{\mathrm{Var}}(\widehat{V}) &= \left(\frac{T-1}{T}\right)^2 \frac{1}{M} \widehat{\mathrm{Var}}(\widehat{s}_j^2) + \left(\frac{M+1}{MT}\right)^2 \frac{2}{M-1} B^2 \\ &+ 2 \frac{(M+1)(T-1)}{M^2 T} \left\{ \widehat{\mathrm{Cov}}(\widehat{s}_j^2, \widehat{\theta}_j^2) - 2 \widehat{\theta} \ \widehat{\mathrm{Cov}}(\widehat{s}_j^2, \widehat{\theta}_j) \right\} \end{split}$$

 $\widehat{\mathrm{Var}}(\widehat{s}_{j}^{2})$ is the sample variance of \widehat{s}_{j}^{2} 's, $j=1,\ldots,M$. $\widehat{\mathrm{Cov}}(\widehat{s}_{j}^{2},\widehat{\theta}_{j}^{2})$ and $\widehat{\mathrm{Cov}}(\widehat{s}_{j}^{2},\widehat{\theta}_{j})$ are the sample covariances of \hat{s}_{i}^{2} 's and $\hat{\theta}_{i}^{2}$'s and \hat{s}_{i}^{2} 's and $\hat{\theta}_{j}$'s, respectively.

Brooks and Gelman (1998) suggested to use the criterion $R_c < 1.2$ for all model parameters to declare MCMC convergence. In practice, a more stringent convergence criterion, $R_c < 1.1$, is often used. If a convergence criterion is not met, longer chains or other means for improving the convergence are needed.

References

Balov, N. 2016. Gelman-Rubin convergence diagnostic using multiple chains. The Stata Blog: Not Elsewhere Classified. http://blog.stata.com/2016/05/26/gelman-rubin-convergence-diagnostic-using-multiple-chains/.

-. 2020. Bayesian inference using multiple Markov chains. The Stata Blog: Not Elsewhere Classified. https://blog.stata.com/2020/02/24/bayesian-inference-using-multiple-markov-chains/.

Brooks, S. P., and A. Gelman. 1998. General methods for monitoring convergence of iterative simulations. Journal of Computational and Graphical Statistics 7: 434-455. https://doi.org/10.1080/10618600.1998.10474787.

Gelman, A., and D. B. Rubin. 1992. Inference from iterative simulation using multiple sequences. Statistical Science 7: 457–472. https://doi.org/10.1214/ss/1177011136.

Also see

[BAYES] bayes — Bayesian regression models using the bayes prefix

[BAYES] bayesmh — Bayesian models using Metropolis-Hastings algorithm

[BAYES] **Bayesian estimation** — Bayesian estimation commands

[BAYES] Bayesian postestimation — Postestimation tools for bayesmh and the bayes prefix

[BAYES] bayesstats summary — Bayesian summary statistics

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