bayesstats grubin — Gelman–Rubin convergence diagnostics

Description

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

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`.

<table>
<thead>
<tr>
<th>options</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sort</td>
<td>list parameters in descending order of their convergence statistics</td>
</tr>
<tr>
<td>skip(#)</td>
<td>skip every # observations from the MCMC sample; default is <code>skip(0)</code></td>
</tr>
<tr>
<td>nolegend</td>
<td>suppress table legend</td>
</tr>
<tr>
<td>display_options</td>
<td>control spacing, line width, and base and empty cells</td>
</tr>
</tbody>
</table>
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()** 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**, **baselevels**, **allbaselevels**, **nofvlabel**, **fvwrap(#)**, **fvwrapon(style)**, and **nolstretch**; see [**R**] Estimation options.

Remarks and examples

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 $R_c$. The parameters with the largest values of $R_c$ 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/r16/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:
  \text{wage} \sim \text{regress}(\text{xb}_\text{wage},\{\text{sigma2}\})

Priors:
\{\text{wage:age }_\text{cons}\} \sim \text{normal}(0,10000) \ (1)
\{\text{sigma2}\} \sim \text{igamma}(0.01,0.01)

(1) Parameters are elements of the linear form \text{xb}_\text{wage}.

Bayesian linear regression
Random-walk Metropolis-Hastings sampling
Number of chains = 3
Per MCMC chain:
  Iterations = 12,500
  Burn-in = 2,500
  Sample size = 10,000
Number of obs = 488
Avg acceptance rate = .3673
Avg efficiency: min = .1409
  avg = .1735
  max = .2294
Avg log marginal-likelihood = -1810.1557
Max Gelman-Rubin \text{Rc} = 1

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>Std. Dev.</th>
<th>MCSE</th>
<th>Median</th>
<th>[95% Cred. Interval]</th>
</tr>
</thead>
<tbody>
<tr>
<td>wage</td>
<td>.4003528</td>
<td>.0599411</td>
<td>.000922</td>
<td>.4002037</td>
<td>.2804134 .5188627</td>
</tr>
<tr>
<td>age</td>
<td>5.999502</td>
<td>1.769855</td>
<td>.026358</td>
<td>6.026288</td>
<td>2.571305 9.517341</td>
</tr>
<tr>
<td>_cons</td>
<td>90.80977</td>
<td>5.822896</td>
<td>.070195</td>
<td>90.49567</td>
<td>79.92114 102.7621</td>
</tr>
</tbody>
</table>

Note: Default priors are used for model parameters.
Note: Default initial values are used for multiple chains.

Compared with example 1 in \text{[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 \{\text{sigma2}\} drops from 0.12 to 0.07.

In the presence of multiple chains, the \text{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.

```plaintext
.bayesstats grubin
Gelman-Rubin convergence diagnostic
Number of chains = 3
MCMC size, per chain = 10,000
Max Gelman-Rubin Rc = 1.000323

<table>
<thead>
<tr>
<th></th>
<th>Rc</th>
</tr>
</thead>
<tbody>
<tr>
<td>wage</td>
<td>1.000062</td>
</tr>
<tr>
<td>_age</td>
<td>1.000323</td>
</tr>
<tr>
<td>_cons</td>
<td>1.000323</td>
</tr>
<tr>
<td>sigma2</td>
<td>1.000253</td>
</tr>
</tbody>
</table>

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}`.

```plaintext
.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

<table>
<thead>
<tr>
<th></th>
<th>Rc</th>
</tr>
</thead>
<tbody>
<tr>
<td>lnsigma2</td>
<td>1.000268</td>
</tr>
</tbody>
</table>

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
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) MCMC sample size of each chain
   r(nchains) number of MCMC chains
   r(Rc_max) 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 $\theta$, let $\{\theta_{jt}\}_{t=1}^T$ be the $j$th simulated chain drawn from the marginal posterior distribution of $\theta$, $j = 1, \ldots, M$. Let $\hat{\theta}_j$ and $\hat{s}_j^2$ be the respective sample posterior mean and variance of the $m$th chain, and let the overall sample posterior mean be $\hat{\theta} = (1/M) \sum_{j=1}^M \hat{\theta}_j$. The between-chains and within-chain variances are given by

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

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

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

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

is an unbiased estimator of the marginal posterior variance of $\theta$.

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

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

They define the so-called “scale” reduction factor as the ratio of $\hat{V}$ and $\sigma^2 = \text{Var}(\theta)$. They further estimate $\sigma^2$ 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:

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

where $\hat{d}$ is the estimated degrees of freedom of the approximating Student’s $t$ distribution for $\theta$

$$\hat{d} = \frac{2\hat{V}^2}{\text{Var}(\hat{V})}$$

and

$$\text{Var}(\hat{V}) = \left(\frac{T-1}{T}\right)^2 \frac{1}{M} \text{Var}(\hat{s}_j^2) + \left(\frac{M+1}{MT}\right)^2 \frac{2}{M-1} B^2$$

$$+ 2\left(\frac{M+1}{M^2T}\right) \left\{ \text{Cov}(\hat{s}_j^2, \hat{\theta}_j^2) - 2\hat{\theta} \text{Cov}(\hat{s}_j^2, \hat{\theta}_j) \right\}$$

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


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