A Local Version of R-hat to Improve MCMC Convergence Diagnostic
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Overview: has the chain converged?

- Diagnosing convergence of Markov chain Monte Carlo (MCMC) is crucial in Bayesian analysis.
- It is frequent to run multiple chains in parallel with different initial values.
- At convergence, all chains should have a similar distribution.

\[ R = \frac{W + B}{W} \]

\( M \) chains of size \( N \), and \( \theta^{(m,n)} \) the \( n \)th draw from chain \( m \). Comparison of the between-variance \( B \) and the within-variance \( W \) of the chains: if \( \theta^{(1,m)}, s_m^{(1)} \) is the mean and variance of \( \theta^{(n,m)} \), and \( \theta^{(1)} \) the mean of \( \theta^{(m)} \),

\[ R = \frac{W + B}{W} \] with \( B = \frac{1}{M - 1} \sum_{m=1}^{M} (\theta^{(1,m)} - \theta^{(1)}; s_m^{(1)}) \), \( W = \frac{1}{M} \sum_{m=1}^{M} s_m^{(1)} \).

If \( R > 1.01 \) convergence issue detected.

Ways of fooling \( \hat{R} \) and improvements [2]

Two cases where \( \hat{R} \) fails:

- Chains with infinite mean and different locations: \( \hat{R} \approx 1 \) \( \Rightarrow \) Bulk-\( \hat{R} \): \( \hat{R} \) on \( z^{(n,m)} \), the normally transformed ranks of \( \theta^{(m)} \).
- Chains with same mean and different variances: \( \hat{R} \approx 1 \) \( \Rightarrow \) Tail-\( \hat{R} \): \( \hat{R} \) on \( z^{(m,n)} \), the deviations from the median.

\( \hat{R} \) = max(Bulk-\( \hat{R} \), Tail-\( \hat{R} \))

### References


### Densities

Idea: compute \( \hat{R} \) on indicator variables \( \{ \{ \theta^{(n,m)} \leq x \} \in \{0,1\} \} \) for a given \( x \).

Benefits:

- Detects (non-)convergence at different quantiles.
- Bernoulli variables \( \Rightarrow \) all moments exist (no need for ranks).
- Detects many false negatives.

Scalar summary: \( \hat{R}_\infty = \sup_x \hat{R}(x) \)

### Fooling rank-\( \hat{R} \), robustness of \( \hat{R}_\infty \)

Idea: find two distributions such that the variables \( z^{(n,m)} \) and \( \zeta^{(n,m)} \) share the same mean, to fool Bulk-\( \hat{R} \) and Tail-\( \hat{R} \) at the same time \( \Rightarrow \) Rank-\( \hat{R} \) < 1.01, and \( \hat{R}_\infty > 1.01 \).

Uniform and Normal densities

### Replications of Rank-\( \hat{R} \) and \( \hat{R}_\infty \)

- Two step algorithm for multivariate diagnostic:
  1. Compute the univariate \( \hat{R}_\infty(i) \) separately on each coordinate \( i \).
  2. If \( \hat{R}_\infty(i) < 1.01 \) for all \( i \), compute the multivariate \( \hat{R}_\infty \) to check convergence of the dependence structure.

### Multivariate extension

Idea: compute \( \hat{R} \) on \( \{ \{ \theta^{(n,m)} \leq x_1, \ldots, \theta^{(n,m)} \leq x_d \} \} \).

- Eq. (1) remains valid for \( \hat{R}(x) \) with \( x = (x_1, \ldots, x_d) \).
- Invariance to reparameterization: if margins are equal, we can assume uniform margins and compute \( \hat{R}(x) \) on \( M \) copulas.

### Upper bound in the multivariate case

Denote by \( R_{i,k} \) the value of \( R_{i,k} \) for \( C_1 \) and \( C_2 \) (\( M = 2 \)). Let \( W_i \) and \( M_i \) Fréchet–Hoeffding copulas in dimension \( d \):

\[ W_i(u) \leq C_i(u) \leq M_i(u), \forall u \in [0,1]^d. \]

Then

\[ R_{i,k} \leq R_{i,k}(W_i, M_i) = \frac{d + 1}{2}. \]