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.

\[ \hat{R} \text{: Potential Scale Reduction Factor [1]} \]

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

with

\[ \hat{B} = \frac{1}{M - 1} \sum_{m=1}^{M} (\hat{\theta}^{(m)} - \bar{\theta})^2, \]

\[ \hat{W} = \frac{1}{M} \sum_{m=1}^{M} s_{m}. \]

If \( \hat{R} > 1.01 \) convergence issue detected.

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

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

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

\[ \text{Rank}-\hat{R} = \max(\text{Bulk}-\hat{R}, \text{Tail}-\hat{R}) \]

A local version of \( \hat{R} \)

\[ \hat{R}(x) \]

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

Benefits:

- Detects (non-)convergence at different quantiles.
- Bernoulli variables \( \implies \) 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 \( C^{(n,m)} \) share the same mean, to fool Bulk-\( \hat{R} \) and Tail-\( \hat{R} \) at the same time \( \implies \) Rank-\( \hat{R} < 1.01 \), and \( \hat{R}_{\infty} > 1.01 \).

Uniform and Normal densities \( \rightarrow \) Replications of Rank-\( \hat{R} \) and \( \hat{R}_{\infty} \)

Multivariate extension

Idea: compute \( \hat{R} \) on \( \{ \theta_1^{(m,n)} \leq x_1, \ldots, \theta_d^{(m,n)} \leq x_d \} \).

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

\[ \Rightarrow \] 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.

\[ \text{Upper bound in the multivariate case} \]

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

\[ W_d(u) \leq C_1(u) \leq M_d(u), \forall u \in [0,1]^d. \]

Then

\[ R_{\infty}(C_1, C_2) \leq R_{\infty}(W_d, M_d) = \sqrt{d + 1}. \]

References