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Discussion of the paper “Rank-Normalization, Folding, and Localization: An Improved $\hat{R}$ for Assessing Convergence of MCMC” by Vehtari et al.

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Abstract: In this note, we discuss an adaptation of the quantile transformation introduced in Vehtari et al. (2021) to the computation of some new $\hat{R}$ and analyse associated theoretical properties.

We have highly appreciated this contribution to improve MCMC convergence diagnostics and would like to thank the authors for their insightful paper. In this note we discuss an adaptation of the quantile transformation introduced in Vehtari et al. (2021) to the computation of some new $\hat{R}$ and analyse associated theoretical properties. More specifically, we propose to compute a continuous version $\hat{\theta}$ of Bernoulli random variables $I(\hat{\theta}(n,m) \leq x)$, rather that on the parameter values $\theta(n,m)$ themselves or their Gaussian version, see Equation (4.1) in Vehtari et al. (2021). This provides us with a function $\hat{R}(x)$ defining a local convergence diagnostic for any $x$. The rank-normalization step is circumvented since working on Bernoulli random variables $I(\theta(n,m) \leq x)$ ensures the existence of all moments whatever the $\theta(n,m)$ distribution is. Assume that all elements $\theta(m,1), \ldots, \theta(m,N)$ of a given chain $m$ follow the same distribution $F_m$ (without independence assumption) which may vary with $m$. Under this stationarity assumption, mean and variance of Bernoulli random variables $I(\theta(n,m) \leq x)$ can be easily written as functions of $F_m$, leading to an explicit expression for $R^2(x)$, the population version of $\hat{R}(x)$:

$$R^2(x) = 1 + \frac{1}{M} \sum_{i=1}^{M} \sum_{j=i+1}^{M} (F_i(x) - F_j(x))^2 \sum_{i=1}^{M} F_i(x)(1 - F_i(x)).$$

(1)

Clearly, $R^2(x) \geq 1$ for all $x \in \mathbb{R}$, with equality iff all $F_m$ coincide. Moreover, $R^2(x) \to 1$ as $|x| \to \infty$. In order to condense the continuous index (1) into a scalar one, we may also consider its supremum over $\mathbb{R}$, denoted by $R_\infty$, which is computed in practice at empirical quantiles. Hereafter, we illustrate how the problems of traditional $\hat{R}$ referred to as items 1. and 2. of Section 1.2 in Vehtari et al. (2021) are bypassed by our proposal on two toy examples. See also Figure 1 for finite sample results.

Example 1: Same mean and different variances. Here $F_m(x) = F(x/\sigma_m)$ where $\sigma_m$ is a scale parameter. As an example, we consider $M$ chains uniformly distributed on $[-\sigma_m, \sigma_m]$ with $\sigma_m = \sigma \leq \sigma_M$ for all $m \in \{1, \ldots, M-1\}$ to model a lack of convergence. From (1), function $R^2$ has a maximum reached at $-\sigma/2$ and $\sigma/2$:

$$R^2_\infty := \sup_{x \in \mathbb{R}} R^2(x) = R^2(\pm \sigma/2) = 1 + \frac{M - 1}{M} \left( \frac{2}{1 + \frac{\sigma_M}{\sigma}} \right).$$

It appears that $R^2_\infty$ is an increasing function of $\sigma_M/\sigma$ with $R^2_\infty = 1$ iff $\sigma_M = \sigma$, and upper bounded by $2 - 1/M$.

Example 2: Heavy tails and different locations. Here $F_m(x) = F(x - \mu_m)$, with $F$ a heavy-tailed distribution and $\mu_m$ a location parameter. We consider Pareto distributed chains with shape parameter $\alpha > 0$, and starting point $\eta > 0$ for $(M-1)$ chains and $\eta_M \geq \eta$ for the remaining one. In that case, $R^2_\infty$ exists for any tail-index $\alpha > 0$:

$$R^2_\infty = R^2(\eta_M) = 1 + \frac{1}{M} \left( \left( \frac{\eta_M}{\eta} \right)^\alpha - 1 \right).$$
Example 1: Unif(−σ/2, σ/2)

Example 2: Pareto(α, η)

Thus, \( R_\infty \) is an increasing function of \( \eta_M / \eta \), with \( R_\infty = 1 \) iff \( \eta_M = \eta \).

To conclude, it appears on these two examples that the proposed local version \( \hat{R}(x) \) allows both to localize the convergence of the MCMC in different quantiles of the distribution, and at the same time to handle the problems not detected by classical \( \hat{R} \) pointed out in the article. Compared to the rank-\( \hat{R} \) proposed in Vehtari et al. (2021), our scalar version \( \hat{R}_\infty \) seems to be more conservative (see third row of Figure 1). Further investigation has to be done on a range of real world problems.

References


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