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A Local Version of $\hat{R}$ to Improve MCMC Convergence Diagnostic



Théo Moins¹, Julyan Arbel¹, Stéphane Girard¹, Anne Dutfoy²

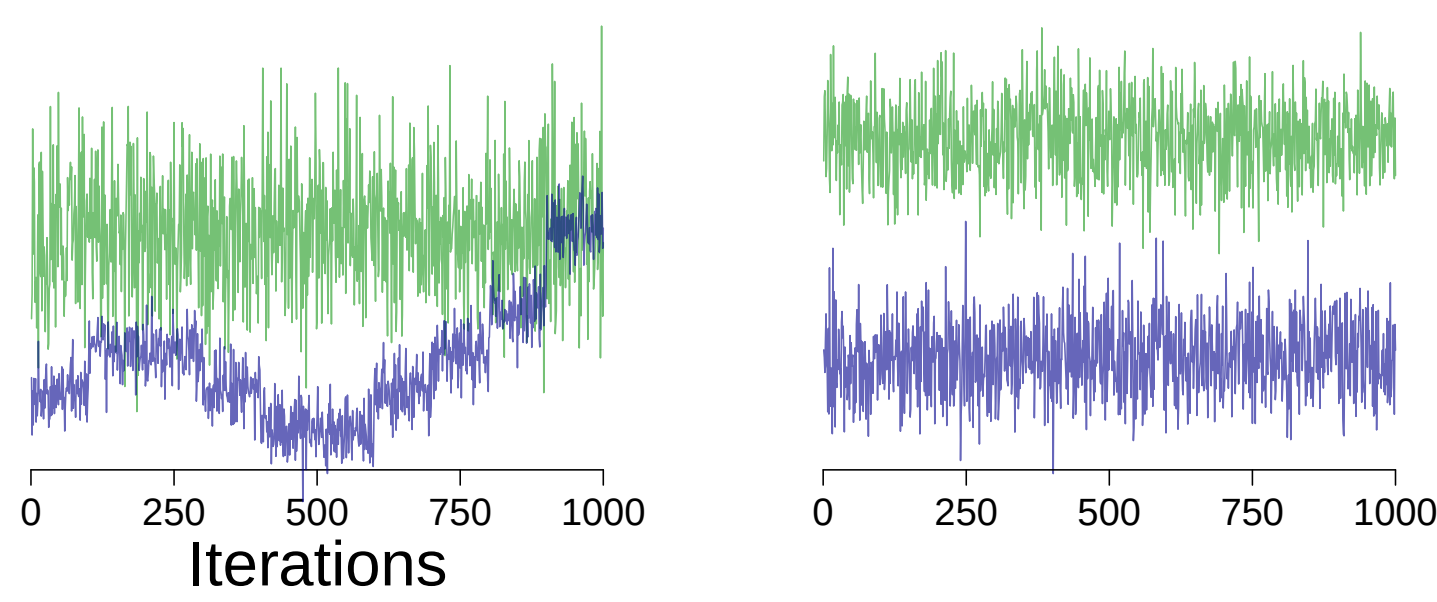
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Overview: has the chain converged?

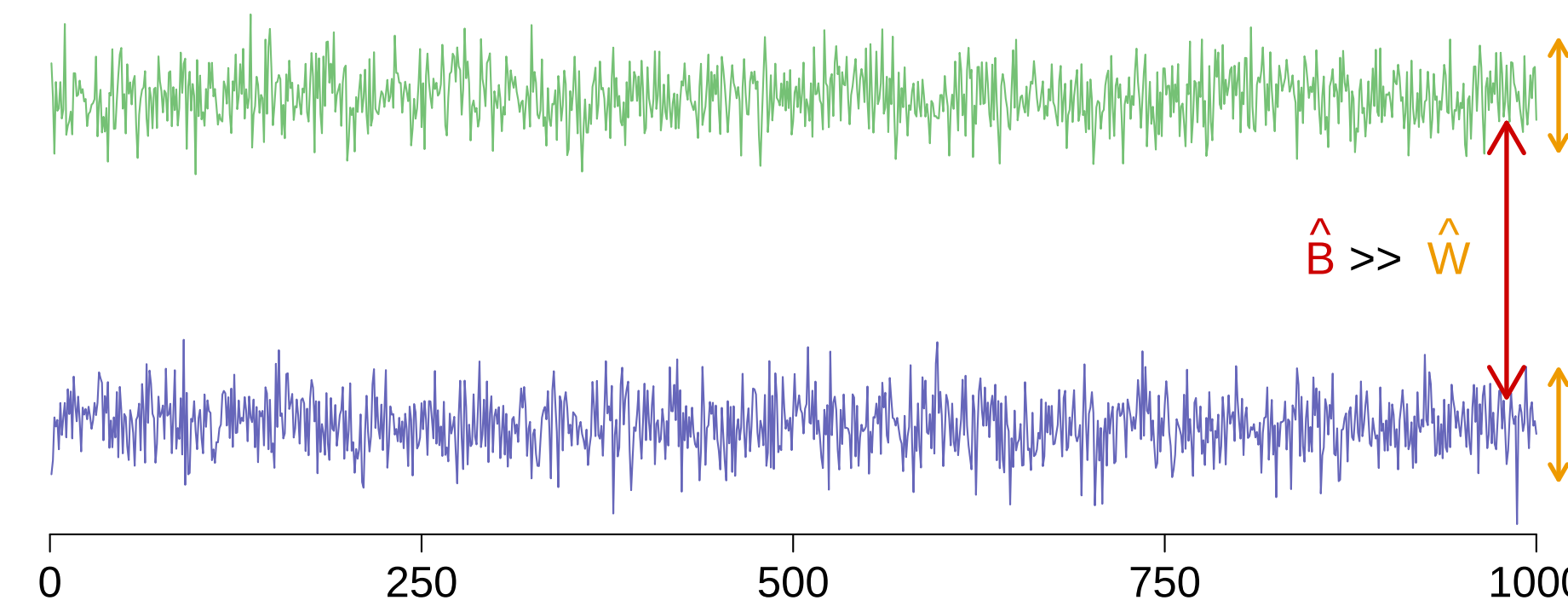
- Diagnosing convergence of Markov chain Monte Carlo (MCMC) is crucial in Bayesian analysis.
- It is frequent to run multiple chains in parallel with different initial values.
- At convergence, all chains should have a similar distribution.



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

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 $(\bar{\theta}^{(\cdot,m)}, s_m^2)$ is the mean and variance of $\theta^{(n,m)}$, and $\bar{\theta}^{(\cdot,\cdot)}$ the mean of $\bar{\theta}^{(\cdot,m)}$,

$$\hat{R} = \sqrt{\frac{\hat{W} + \hat{B}}{\hat{W}}}, \quad \text{with} \quad \begin{cases} \hat{B} = \frac{1}{M-1} \sum_{m=1}^M (\bar{\theta}^{(\cdot,m)} - \bar{\theta}^{(\cdot,\cdot)})^2, \\ \hat{W} = \frac{1}{M} \sum_{m=1}^M s_m^2. \end{cases}$$



If $\hat{R} > 1.01$: convergence issue detected.

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

Two cases where $\hat{R}$ fails:

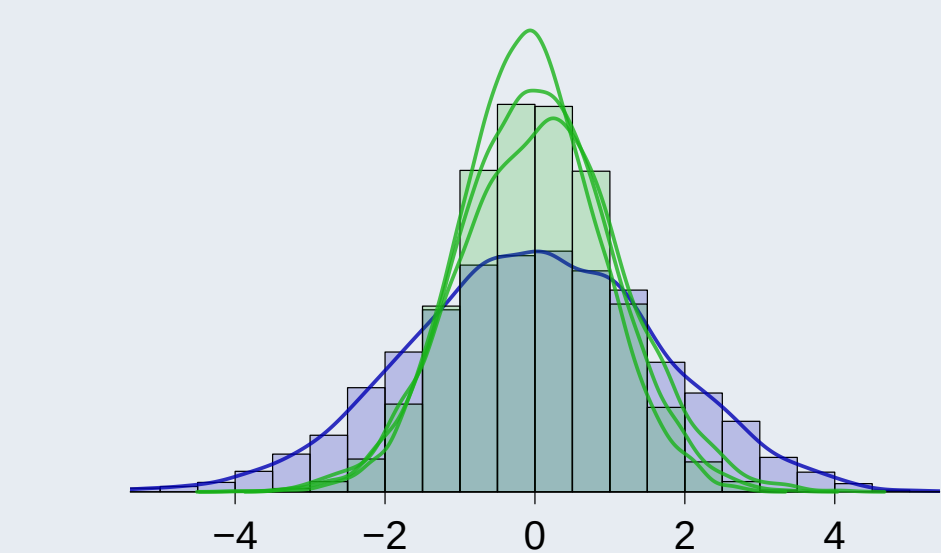
- Chains with infinite mean and different locations: $\hat{R} \approx 1$
 $\hookrightarrow$ **Bulk- $\hat{R}$** : $\hat{R}$ on $z^{(n,m)}$, the normally transformed ranks of $\theta^{(m,n)}$.
- Chains with same mean and different variances: $\hat{R} \approx 1$
 $\hookrightarrow$ **Tail- $\hat{R}$** :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

$\Downarrow$

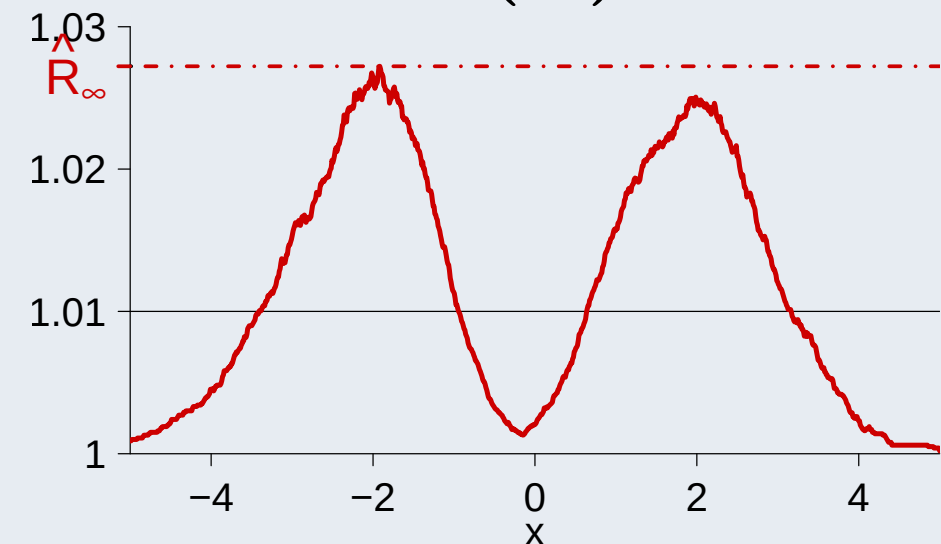
$$\text{Rank-}\hat{R} = \max(\text{Bulk-}\hat{R}, \text{Tail-}\hat{R})$$

A local version of $\hat{R}$

Densities



$\hat{R}(x)$



Idea: compute $\hat{R}$ on indicator variables $\mathbb{I}\{\theta^{(n,m)} \leq x\} \in \{0, 1\}$ 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: $\hat{R}_\infty = \sup_x \hat{R}(x)$

Population version

Assume chain m has stationary distribution F_m .

As $\mathbb{E}[\mathbb{I}\{\theta^{(n,m)} \leq x\}] = F_m(x)$, and $\text{Var}[\mathbb{I}\{\theta^{(n,m)} \leq x\}] = F_m(x) - F_m^2(x)$, theoretical within-variance $W(x)$ and between-variance $B(x)$ are

$$W(x) = \frac{1}{M} \sum_{m=1}^M (F_m(x) - F_m^2(x)), \quad B(x) = \frac{1}{M} \sum_{m=1}^M F_m^2(x) - \left(\frac{1}{M} \sum_{m=1}^M F_m(x) \right)^2.$$

$\implies$ Population version of $\hat{R}(x)$ is

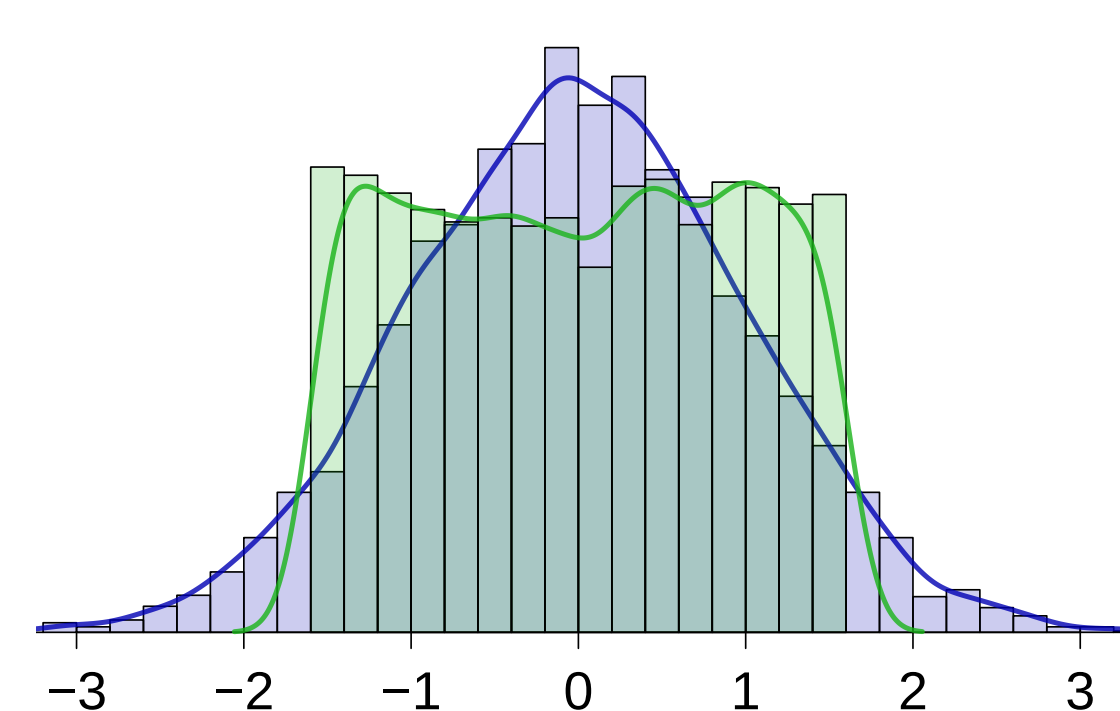
$$R(x) := \sqrt{\frac{W(x) + B(x)}{W(x)}} = \sqrt{1 + \frac{\frac{1}{M} \sum_{i=1}^M \sum_{j=i+1}^M (F_i(x) - F_j(x))^2}{\sum_{i=1}^M F_i(x)(1 - F_i(x))}}. \quad (1)$$

Properties: $R \geq 1$, and $R \equiv 1 \iff$ all F_m are equal,
 R_∞ invariant with respect to reparameterisation.

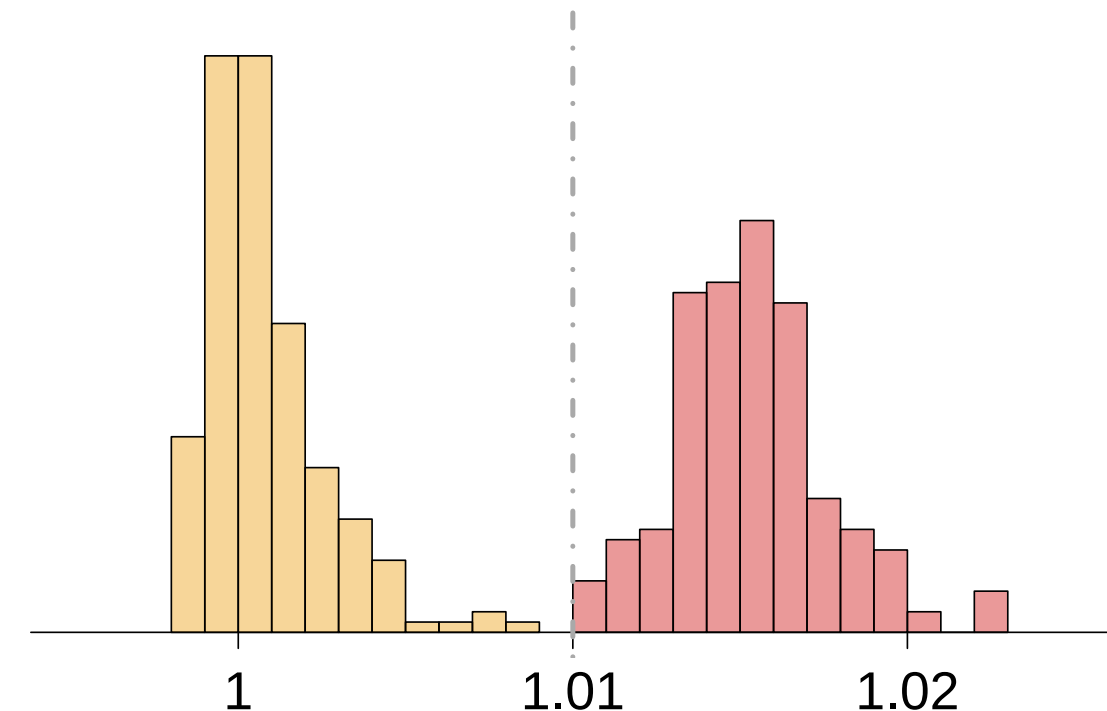
Fooling rank- $\hat{R}$, robustness of $\hat{R}_\infty$

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 $\implies \text{Rank-}\hat{R} < 1.01$, and $\hat{R}_\infty > 1.01$.

Uniform and Normal densities



Replications of Rank- $\hat{R}$ and $\hat{R}_\infty$



Threshold elicitation

Assume all $\hat{F}_j \rightarrow F$ with a Markov chain central limit theorem:

$$\sqrt{nm}(\hat{F}(x) - F(x)) \xrightarrow{d} \mathcal{N}(0, \sigma^2(x)), \quad \hat{F}(x) = \frac{1}{nm} \sum_{j=1}^m \sum_{i=1}^n \mathbb{I}\{\theta^{(i,j)} \leq x\}$$

Define $\text{ESS}(x) := nm \frac{F(x)(1 - F(x))}{\sigma^2(x)}$. Then for any $x \in \mathbb{R}$,

$$\text{ESS}(x)(\hat{R}^2(x) - 1) \xrightarrow{d} \chi_{m-1}^2 \quad \text{as } n \rightarrow \infty.$$

$$R_{\text{lim},\alpha}(x) := \sqrt{1 + \frac{z_{m-1,1-\alpha}}{\text{ESS}(x)}} \implies \mathbb{P}(\hat{R}(x) \geq R_{\text{lim},\alpha}(x)) \simeq \alpha.$$

With $\alpha = 0.05$, $m = 4$, $\text{ESS}(x) = 400$: $R_{\text{lim},\alpha}(x) \approx 1.010$

Multivariate extension

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

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

$\hookrightarrow$ Two-step algorithm for multivariate diagnostic:

- Compute the univariate $\hat{R}_{\infty,i}$ separately on each coordinate i .
- If $\hat{R}_{\infty,i} < 1.01$ for all i , compute the multivariate $\hat{R}_\infty$ to check convergence of the dependence structure.

Upper bound in the multivariate case

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

$$W_d(\mathbf{u}) \leq C_i(\mathbf{u}) \leq M_d(\mathbf{u}), \forall \mathbf{u} \in [0, 1]^d.$$

Then

$$R_\infty(C_1, C_2) \leq R_\infty(W_d, M_d) = \sqrt{\frac{d+1}{2}}.$$

References

- [1] A. Gelman and D. Rubin. Inference from iterative simulation using multiple sequences. *Statistical Science*, 7(4):457–472, 1992.
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