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Improving MCMC convergence diagnostic: a local version of \hat{R}



Théo Moins¹, Julyan Arbel¹, Stéphane Girard¹, Anne Dutfoy²

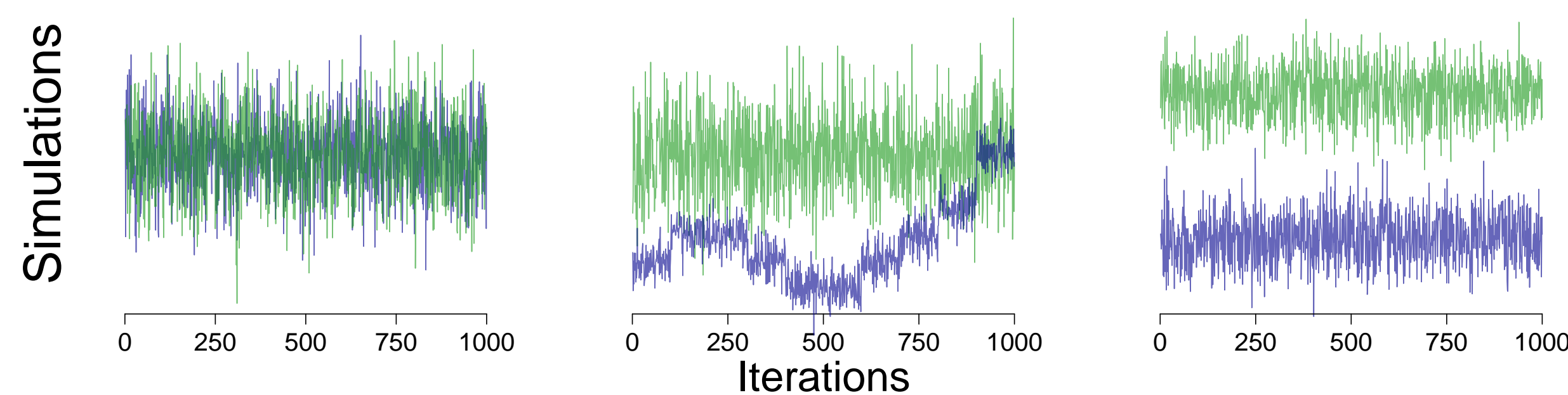
¹Statify, Inria Grenoble Rhône-Alpes,

²EDF R&D dept. Périclès



Overview: has the chain converged?

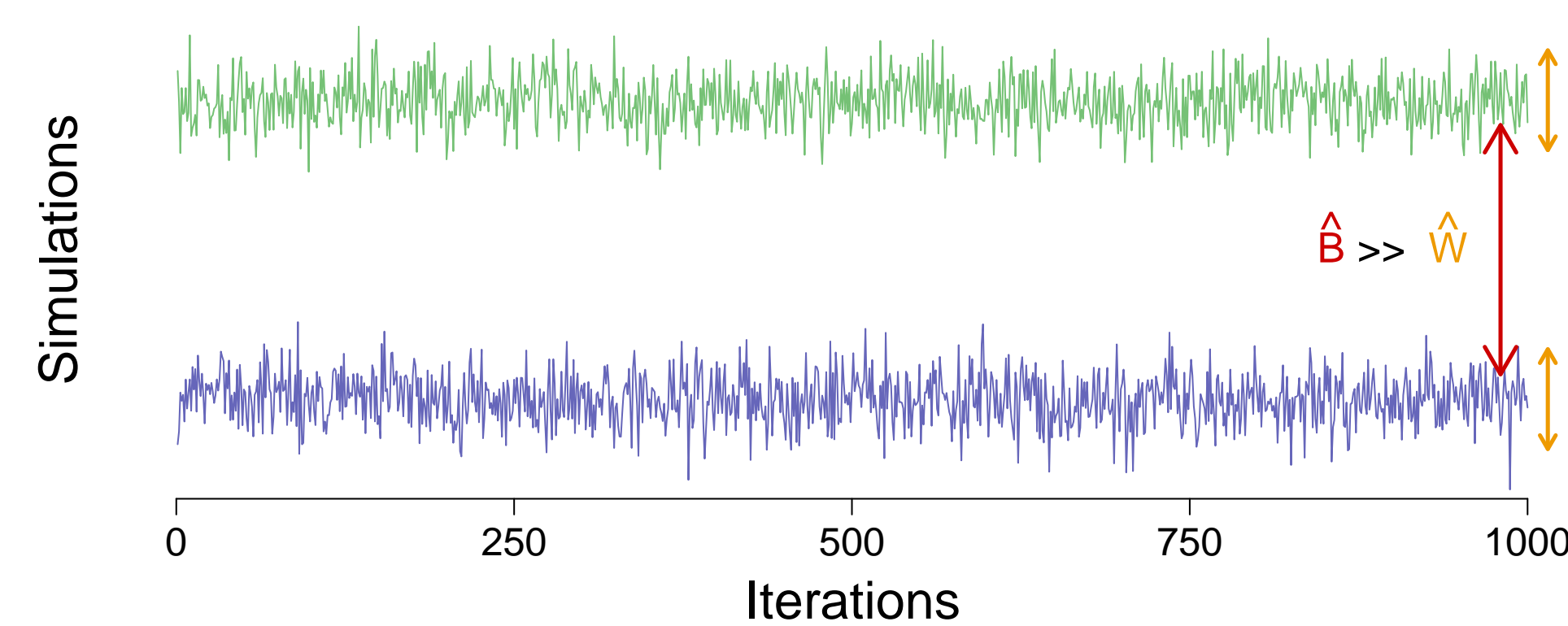
- Diagnosing convergence of Markov chain Monte Carlo (MCMC) is crucial in Bayesian analysis.
- It is frequent to run multiple chains in parallel with different initial values.
- At convergence, all chains should have a similar distribution.



\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 $\bar{\theta}^{(\cdot)}$ the mean of $\bar{\theta}^{(\cdot,m)}$,

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

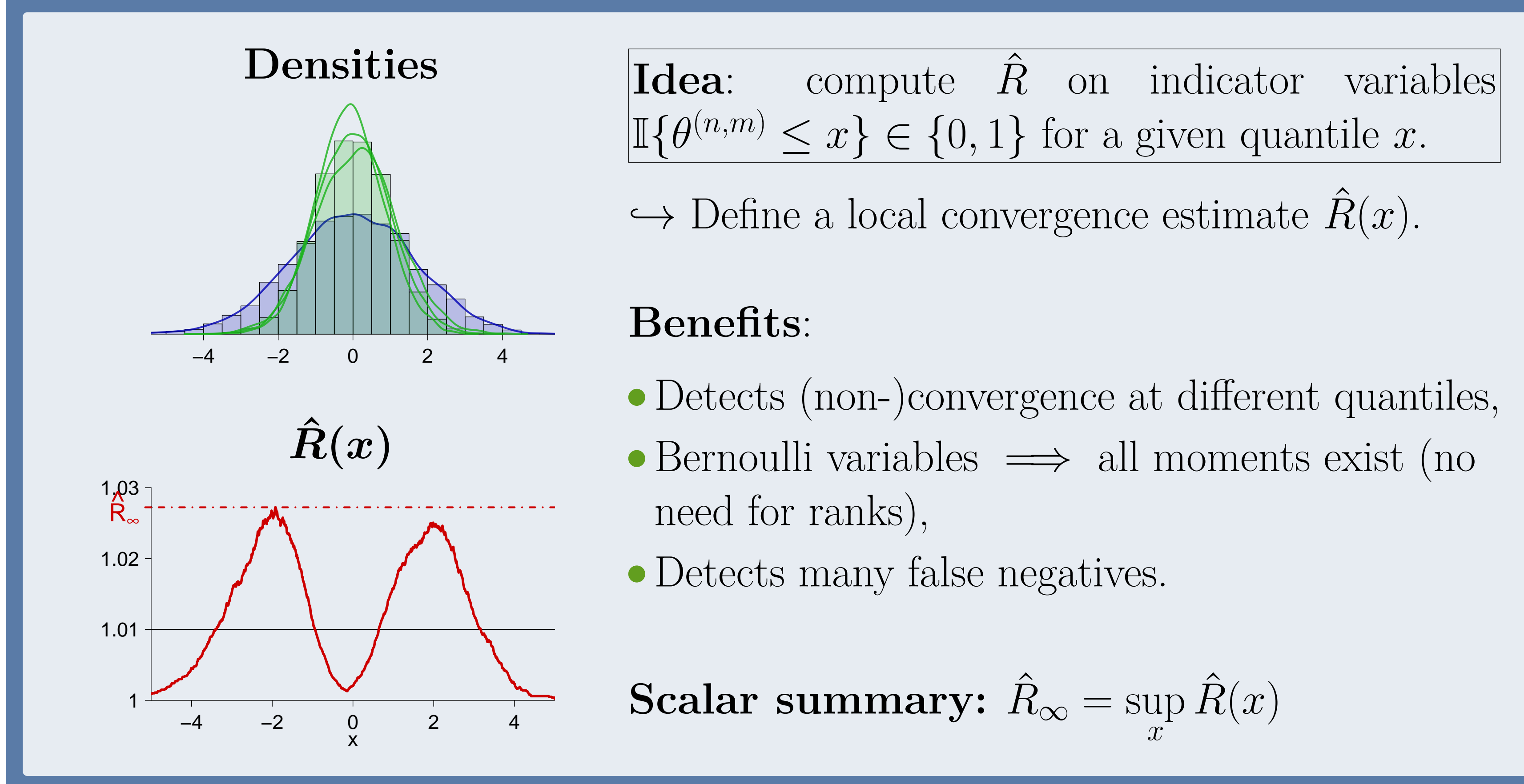


If $\hat{R} > 1.01$: convergence issue detected.

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

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

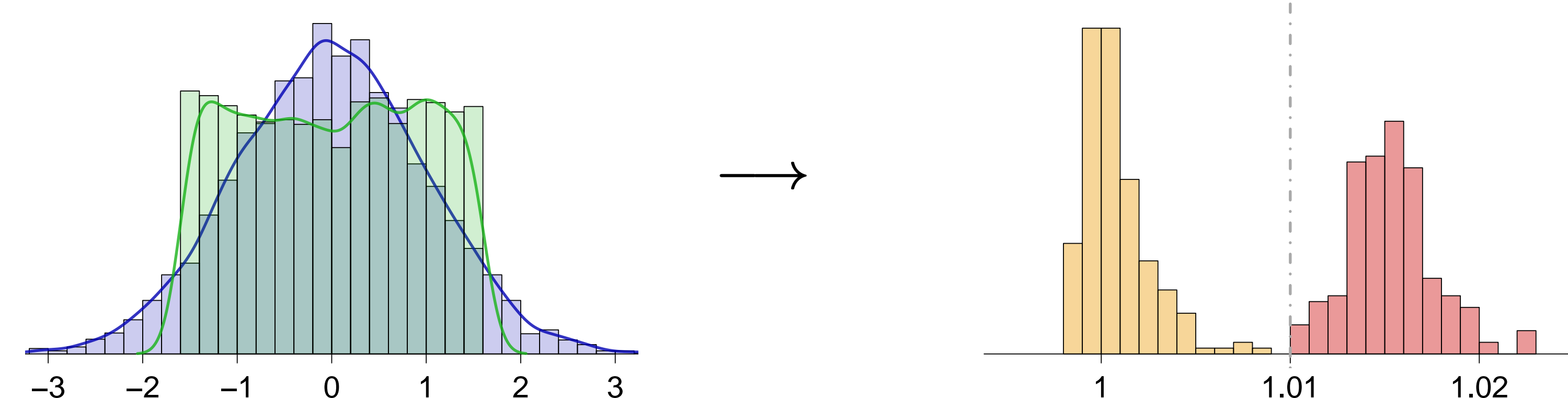
A local version of \hat{R}



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

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

Uniform and Normal densities 200 replications of Rank- \hat{R} and \hat{R}_∞



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

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

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

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

Properties:

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

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 (instead of M CDFs).

\hookrightarrow 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}_∞ to check convergence of the dependence structure.

- With $M = 2$, copulas C_1 and C_2 and $\mathbf{u} \in [0, 1]^d$:

$$R(\mathbf{u}) = \sqrt{1 + \frac{1}{2} \frac{(C_1(\mathbf{u}) - C_2(\mathbf{u}))^2}{C_1(\mathbf{u})(1 - C_1(\mathbf{u})) + C_2(\mathbf{u})(1 - C_2(\mathbf{u}))}}.$$

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 (C_-, C_+) two bounding copulas:

$$\begin{cases} C_-(\mathbf{u}) \leq C_1(\mathbf{u}) \leq C_+(\mathbf{u}) \\ C_-(\mathbf{u}) \leq C_2(\mathbf{u}) \leq C_+(\mathbf{u}) \end{cases} \quad \forall \mathbf{u} \in [0, 1]^d.$$

Then

$$R_\infty(C_1, C_2) \leq R_\infty(C_-, C_+).$$

Corollary: if W_d and M_d are the lower and upper Fréchet-Hoeffding copulas in dimension d ,

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

References

- [1] A. Gelman and D. Rubin. Inference from iterative simulation using multiple sequences. *Statistical Science*, 7(4):457–472, 1992.
- [2] A. Vehtari, A. Gelman, D. Simpson, B. Carpenter, and P.-C. Bürkner. Rank-Normalization, Folding, and Localization: An Improved \hat{R} for Assessing Convergence of MCMC. *Bayesian Analysis*, 2021.
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