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

Inria

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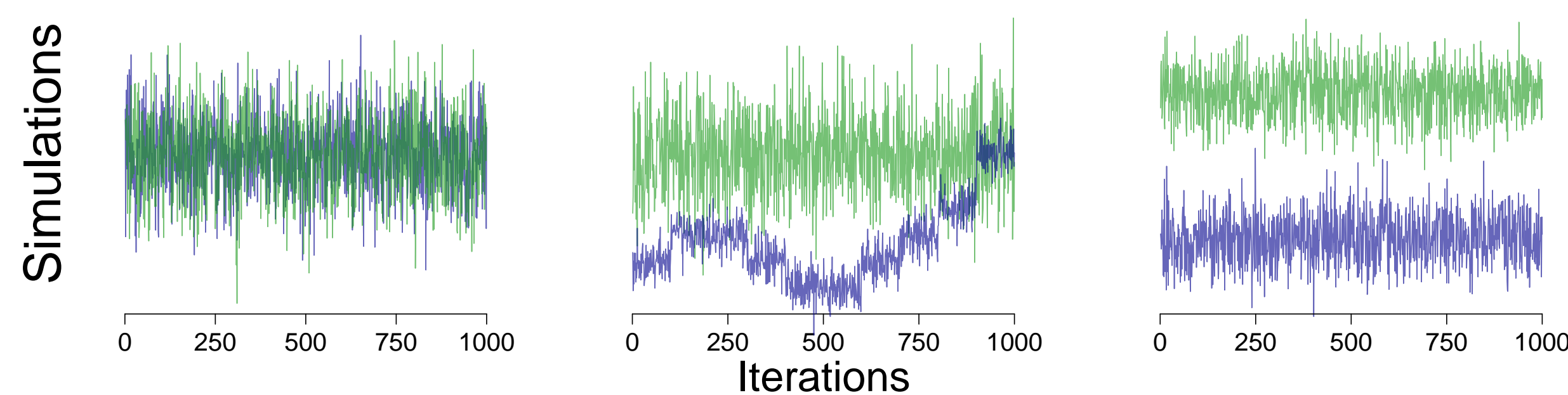
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## Overview: has the chain converged?

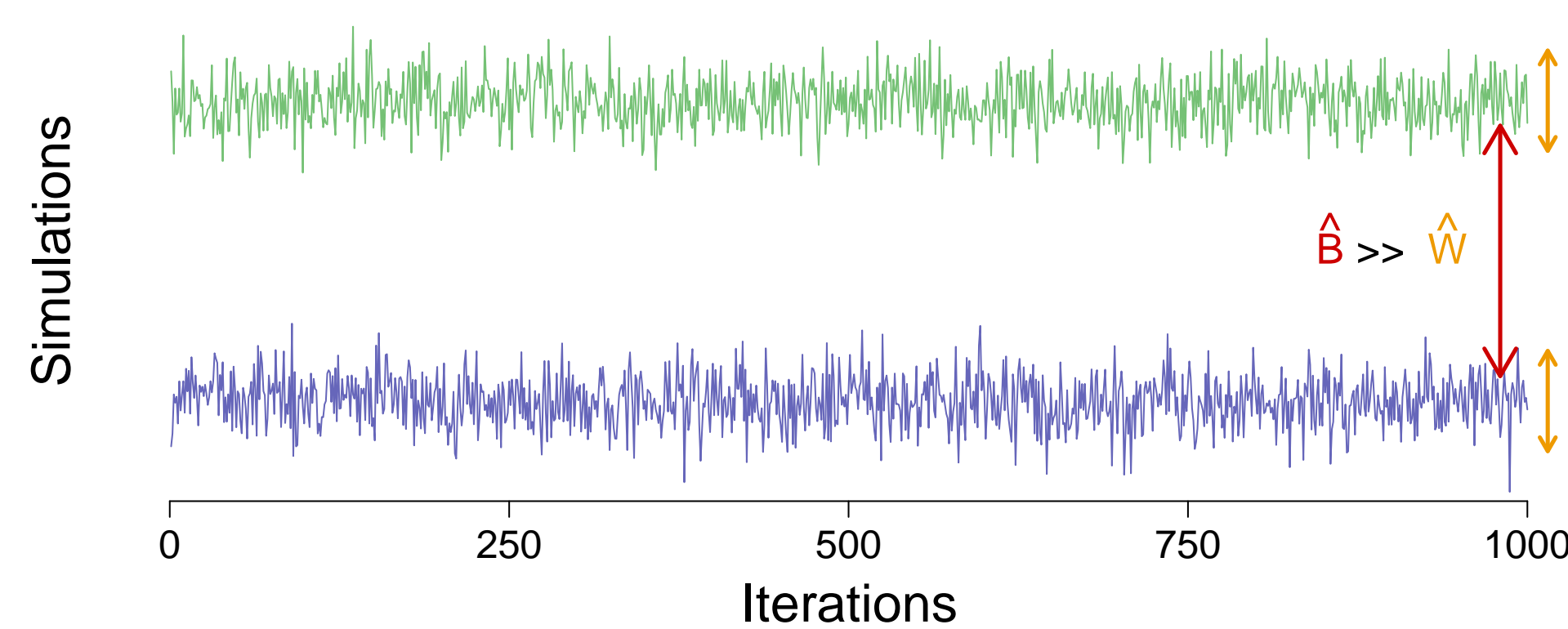
- Diagnosing convergence of Markov chain Monte Carlo (MCMC) is crucial in Bayesian analysis.
- It is frequent to run multiple chains in parallel with different initial values.
- At convergence, all chains should have a similar distribution.



## $\hat{R}$ : 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  $\bar{\theta}^{(\cdot)}$  the mean of  $\bar{\theta}^{(\cdot,m)}$ ,

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

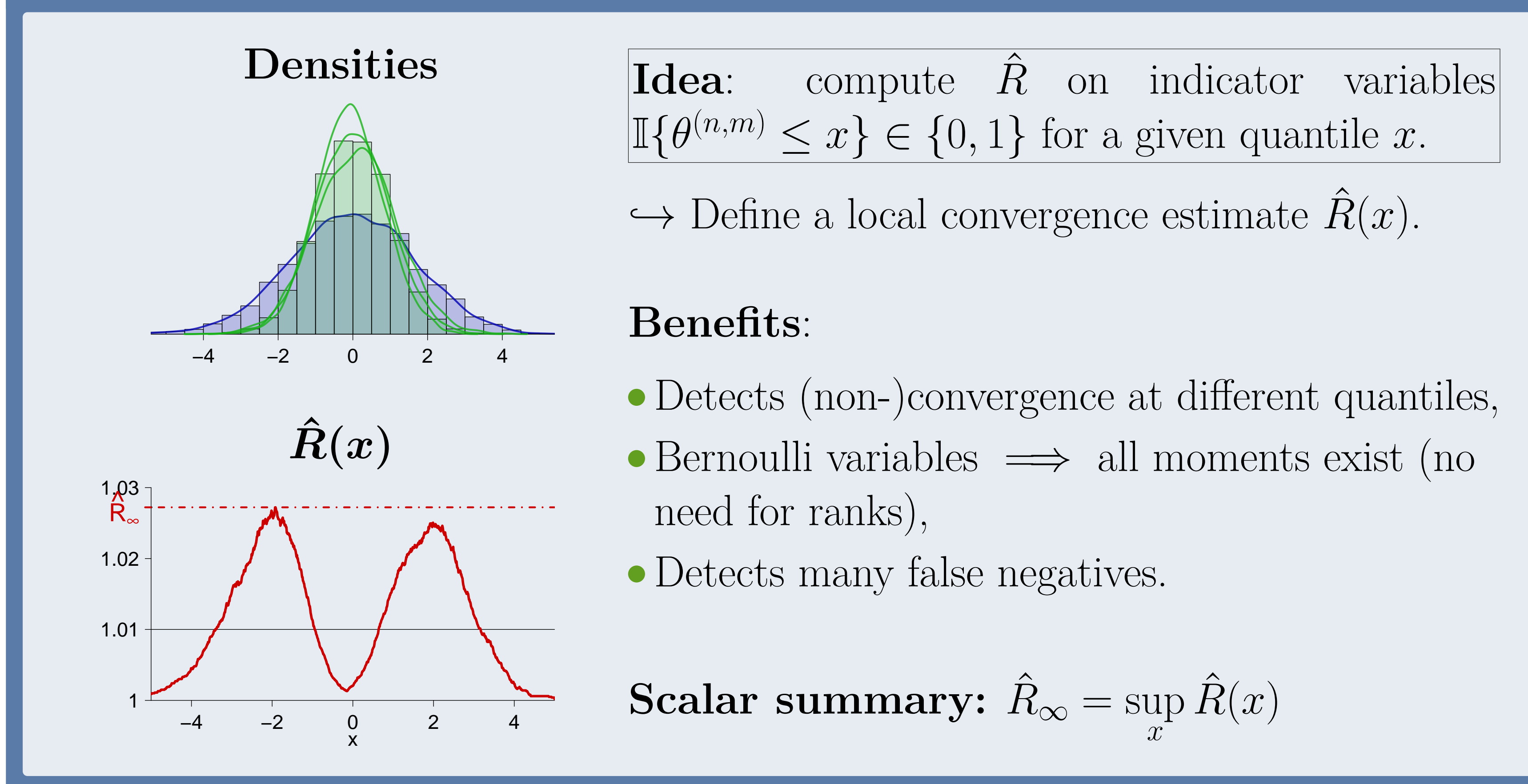


If  $\hat{R} > 1.01$ : convergence issue detected.

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

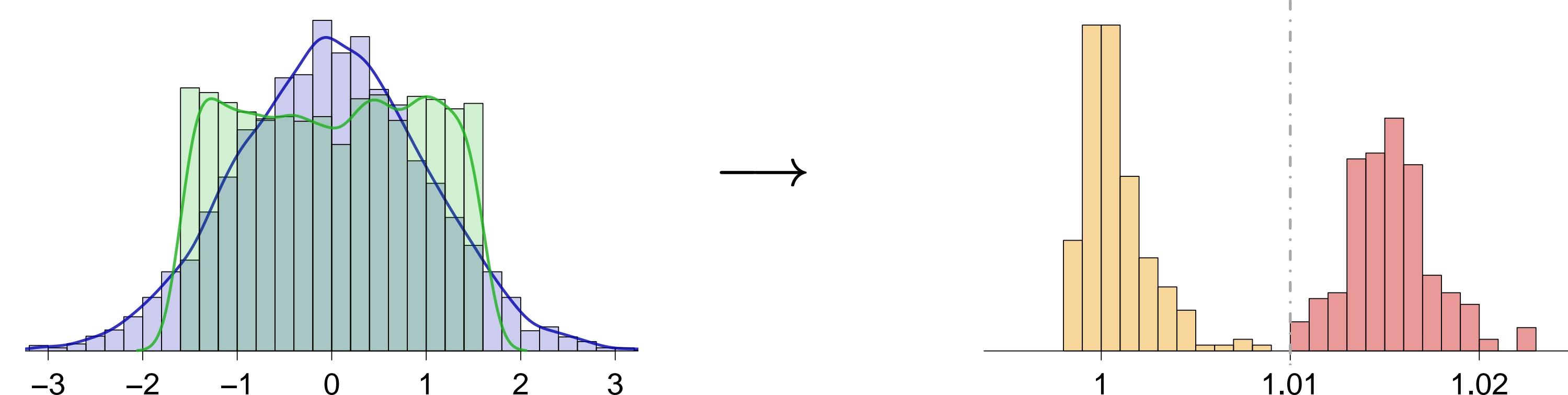
## A local version of $\hat{R}$



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

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

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



## 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,
  - $R_\infty$  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  $\hat{R}_\infty$  to check convergence of the dependence structure.

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

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

## Upper bound in the multivariate case

Denote by  $R_\infty(C_1, C_2)$ , the value of  $R_\infty$  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.
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