On the use of a local $\hat{R}$ to improve MCMC convergence diagnostic

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Joint with Julyan Arbel[1], Anne Dutfoy[2] Stéphane Girard[1]

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Context

Limits of extrapolation associated with Bayesian extreme value models.

Aim: Understand the risks of hazardous meteorological events.

Inondations : le Lot-et-Garonne touché par la "crue la plus importante depuis quarante ans"
(Source: lemonde.fr, Février 2021)

MCMC

Bayesian inference on $\theta \sim \pi \implies$ computation of $\mathbb{E}_\pi[f(\theta)] = \int f(\theta)\pi(\theta)d\theta$.

MCMC (Markov Chain Monte Carlo):

Monte Carlo	Markov Chain
$\mathbb{E}[f(\theta)] \approx \frac{1}{n}\sum_{i=1}^n f(\theta_i)$	$\theta_{i+1} \mid \theta_i \sim P(\theta_i, \cdot)$

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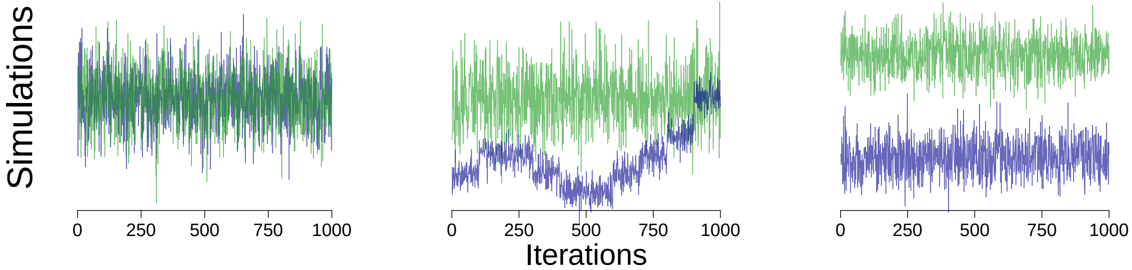
- **Algorithms**: Metropolis–Hastings, Gibbs sampling, Hamiltonian Monte Carlo (HMC) (Neal, 2011), No U-Turn Sampler (NUTS) (Hoffman and Gelman, 2014), etc.
- **Librairies**: JAGS (Plummer et al., 2003), Stan (Carpenter et al., 2017), PyMC3 (Salvatier et al., 2016)...

Has the chain(s) converged? Need for multiple chains



$\hat{R}$ (aka potential scale reduction factor)

Introduced by Gelman and Rubin (1992).

Consider m chains of size n, with $\theta^{(i,j)}$ denoting the ith draw from chain j.

Comparison of the **between-variance** B and the **within-variance** W of the chains:

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$$\text{Between var}: \hat{B} = \frac{1}{m-1}\sum_{j=1}^{m}(\bar{\theta}^{(.,j)} - \bar{\theta}^{(.,.)})^2, \quad \text{where } \bar{\theta}^{(.,j)} = \frac{1}{n}\sum_{i=1}^{n}\theta^{(i,j)}, \quad \bar{\theta}^{(.,.)} = \frac{1}{m}\sum_{j=1}^{m}\bar{\theta}^{(.,j)},$$

$$\text{Within var}: \hat{W} = \frac{1}{m}\sum_{j=1}^{m}s_j^2, \quad \text{where } s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\theta^{(i,j)} - \bar{\theta}^{(.,j)})^2.$$

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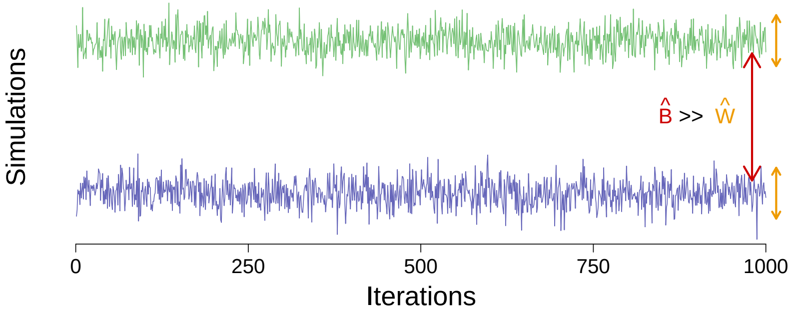

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Inference from iterative simulation using multiple sequences
A Gelman, DB Rubin - Statistical science, 1992 - projecteuclid.org
The Gibbs sampler, the algorithm of Metropolis and similar iterative simulation methods are potentially very helpful for summarizing multivariate distributions. Used naively, however, iterative simulation can give misleading answers. Our methods are simple and generally …
Cited by 13999 Related articles All 20 versions Import into BibTeX

Recent improvement: rank-$\hat{R}$ Vehtari et al. (2021)

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Local version of $\hat{R}$, or $\hat{R}(x)$

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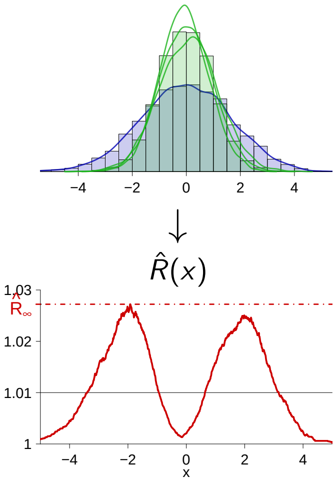

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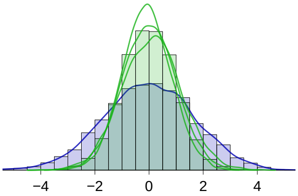
Idea: compute $\hat{R}$ on indicator variables $\mathbb{I}(\theta^{(i,j)} \leq x) \in \{0,1\}$ for a given quantile x

Benefits:

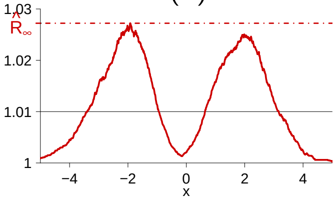
- It is local
  $\implies$ detects (non-)convergence locally
- Bernoulli variables
  $\implies$ all moments exist (no need for ranks)
- Detects many false negatives
- Scalar summary:

$$\hat{R}_\infty = \sup_x \hat{R}(x)$$



$\downarrow$

$\hat{R}(x)$



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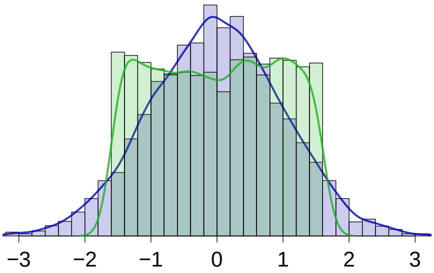
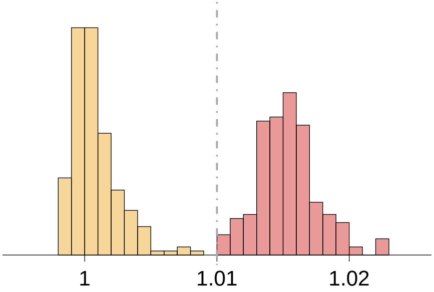
$\hat{R}_\infty$ where Rank-$\hat{R}$ is fooled

Uniform and Normal densities



$\rightarrow$

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



https://theomoins.github.io/localrhat/Simulations.html

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Theoretical properties

Assume chain $Z = j$ has distribution F_j (stationarity assumption, to focus on mixing). Then,

$$\mathbb{E}[I(\theta \leq x) \mid Z = j] = F_j(x), \quad \text{and} \quad \mathrm{Var}\left[I(\theta \leq x) \mid Z = j\right] = F_j(x) - F_j^2(x)$$

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Theoretical $B(x)$ and $W(x)$:

$$B(x) = \frac{1}{m}\sum_{j=1}^{m} F_j^2(x) - \left(\frac{1}{m}\sum_{j=1}^{m} F_j(x)\right)^2, \qquad W(x) = \frac{1}{m}\sum_{j=1}^{m} \left(F_j(x) - F_j^2(x)\right).$$

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Proposition (Moins et al., 2022)

$R(x)$, the population version of $\hat{R}(x)$, can be written

$$R(x) := \sqrt{\frac{W(x) + B(x)}{W(x)}} = \sqrt{1 + \frac{\sum_{j=1}^{m}\sum_{k=j+1}^{m}\left(F_k(x) - F_j(x)\right)^2}{m\sum_{j=1}^{m} F_j(x)(1 - F_j(x))}}.$$

Population $R(x)$

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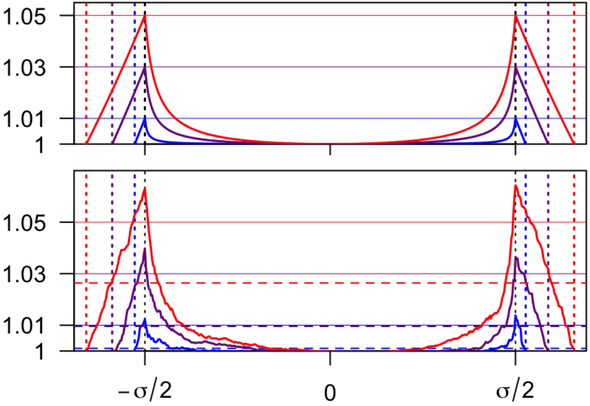

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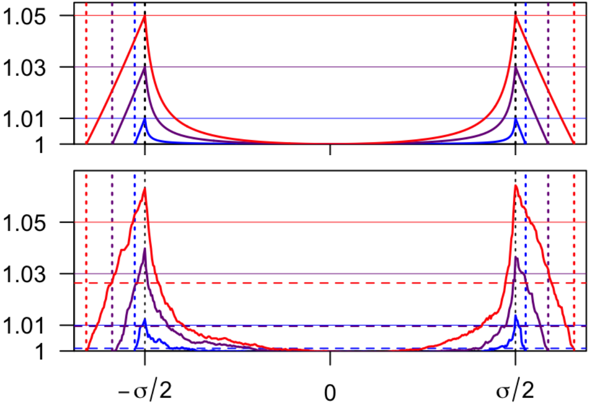
Properties:

- $R \equiv 1 \iff$ all F_j are equal
- $R \geq 1$
- $\lim_{\pm\infty} R = 1$
- R_∞ invariant to monotone transformation



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Convergence properties of $\hat{R}(x)$

Assumption of a Markov chain central limit theorem:

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

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$\hookrightarrow$ Number of samples to obtain the same variance in the i.i.d case.

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Proposition (Moins et al., 2022)

Assume that all m chains are mutually independent and have converged to a common distribution F. Then for any $x \in \mathbb{R}$,

$$\mathrm{ESS}(x)(\hat{R}^2(x) - 1) \xrightarrow{d} \chi^2_{m-1} \quad \text{as} \quad n \to \infty.$$

Threshold elicitation: $\hat{R}(x)$

Let $z_{m-1,1-\alpha}$ be the quantile of level $1-\alpha$ of the χ^2_{m-1} distribution, and introduce the associated threshold (type I error)

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

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$\mathrm{ESS}(x)$	α	m	$R_{\mathrm{lim},\alpha}(x)$
400	0.05	2	1.005
		4	1.010
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$\hookrightarrow$ 1.01 seems reasonable in the most common configurations.

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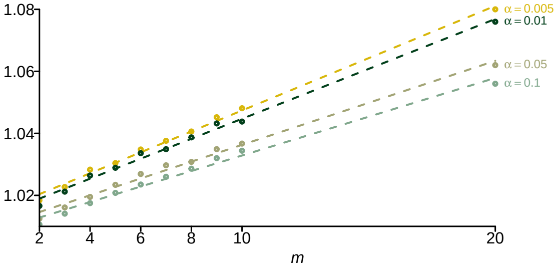
Estimation using replications:

m	0.005	0.01	0.05	0.1
2	1.018	1.016	**1.012**	1.010
3	1.023	1.022	1.016	1.014
4	1.027	1.025	**1.020**	1.018
8	1.038	1.037	**1.031**	1.028
10	1.043	1.041	1.036	1.033
20	1.080	1.076	1.062	1.056



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Preprint! 🎉

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March 7, 2022

Abstract

Diagnosing convergence of Markov chain Monte Carlo is crucial and remains an essentially unsolved problem. Among the most popular methods, the potential scale reduction factor, commonly named $\hat{R}$, is an indicator that monitors the convergence of output chains to a target distribution, based on a comparison of the between- and within-variances. Several improvements have been suggested since its introduction in the 90s. Here, we aim at better understanding the $\hat{R}$ behavior by proposing a localized version that focuses on quantiles of the target distribution. This new version relies on key theoretical properties of the associated population value. It naturally leads to proposing a new indicator $\hat{R}_\infty$, which is shown to allow both for localizing the Markov chain Monte Carlo convergence in different quantiles of the target distribution, and at the same time for handling some convergence issues not detected by other $\hat{R}$ versions.

T. Moins, J. Arbel, A. Dutfoy & S. Girard. (2022+) "*On the use of a local R-hat to improve MCMC convergence diagnostic*" https://hal.inria.fr/hal-03600407/document

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Multivariate case

If parameter θ is d-dimensional: simple multivariate extension by computing $\hat{R}$ on indicator variables $I(\theta_1^{(i,j)} \leq x_1, \ldots, \theta_d^{(i,j)} \leq x_d)$

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If parameter θ is d-dimensional: simple multivariate extension by computing $\hat{R}$ on indicator variables $I(\theta_1^{(i,j)} \leq x_1, \ldots, \theta_d^{(i,j)} \leq x_d)$

As before, population version $R(\boldsymbol{x})$, with $\boldsymbol{x} = (x_1, \ldots, x_d)$:

$$R(\boldsymbol{x}) = \sqrt{1 + \frac{\sum_{j=1}^{m} \sum_{k=j+1}^{m} \left(F_j(\boldsymbol{x}) - F_k(\boldsymbol{x})\right)^2}{m \sum_{j=1}^{m} F_j(\boldsymbol{x})(1 - F_j(\boldsymbol{x}))}}.$$

- $R \equiv 1 \iff$ all F_j are equal
- $R \geq 1$
- R_∞ invariant to monotone transformation $\implies$ if convergence of margins, we can compute R on M copulas (instead of M CDFs)

Multivariate case: upper bound

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Lemma

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

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

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Proposition (Moins et al., 2022)

Let W_d and M_d the lower and upper Fréchet–Hoeffding copulas in dimension d. Then

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

Multivariate case: bound refinement

Fréchet–Hoeffding copula bounds (comonotone random variables):

$$W_d(\boldsymbol{u}) := \max\left\{1 - d + \sum_{i=1}^{d} u_i, 0\right\} \quad \text{and} \quad M_d(\boldsymbol{u}) := \min\{u_1, \ldots, u_d\}.$$

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Let us refine the upper bound by comparing with the independent copula $\Pi_d(\boldsymbol{u}) := \prod_{i=1}^{d} u_i$:

- Positive Lower Orthant Dependence (PLOD) copula:
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⚠ This does not define a total order on copulas!

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Let's stay in the case $m = 2$ chains.

Corollary (Moins et al., 2022)

For any two PLOD d-variate copulas C_1 and C_2, $R_\infty(C_1, C_2) \leq R_\infty(\Pi_d, M_d)$ with

$$\begin{cases} R_\infty(\Pi_2, M_2) = \sqrt{\frac{1}{2} + \frac{1}{\sqrt{3}}} \approx 1.038 & \text{if } d = 2, \\ \sqrt{\frac{d}{2\log d}}(1 + o(1)) \leq R_\infty(\Pi_d, M_d) \leq \sqrt{\frac{d+1}{2}} & \text{as } d \to \infty. \end{cases}$$

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Corollary (Moins et al., 2022)

For any two NLOD d-variate copulas C_1 and C_2, $R_\infty(C_1, C_2) \leq R_\infty(\Pi_d, W_d)$ with

$$R_\infty(\Pi_d, W_d) = \sqrt{1 + \frac{1}{2}\frac{1}{\left(1 - \frac{1}{d}\right)^{-d} - 1}}.$$

Multivariate case: bound refinement

Asymmetric behaviour:

- $R_\infty(\Pi_d, M_d)$ diverges with d at the (almost) same rate as $R_\infty(M_d, W_d)$,
- $R_\infty(\Pi_d, W_d) \xrightarrow[d\to\infty]{} 1.136$.

Illustration with $m = 2$ chains with bivariate normal distributions:

$$\boldsymbol{\theta}^{(i,1)} \sim \mathcal{N}\left(\begin{pmatrix}0\\0\end{pmatrix}, \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\right), \quad \boldsymbol{\theta}^{(i,2)} \sim \mathcal{N}\left(\begin{pmatrix}0\\0\end{pmatrix}, \begin{pmatrix}1 & \rho\\\rho & 1\end{pmatrix}\right), \quad \text{with} \quad \rho \in (-1, 1).$$

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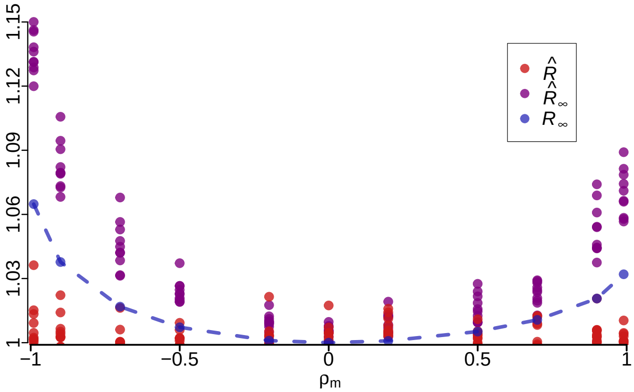

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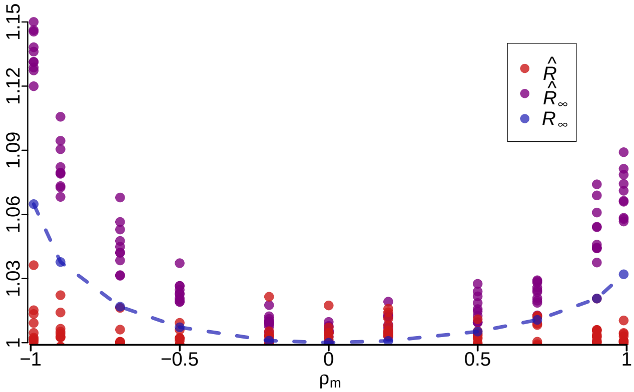

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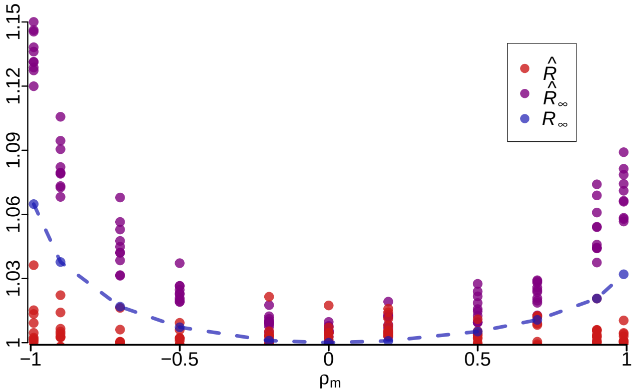

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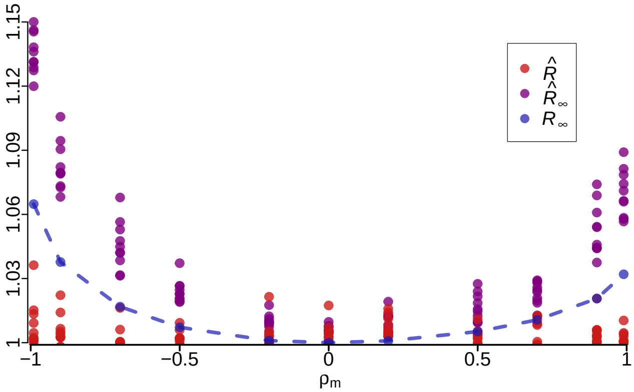

- PLOD and NLOD bounds when $|\rho| \to 1$,
- Asymmetry which favour NLOD when $d = 2$,
- It can be inverted by computing $\hat{R}_\infty^-$ on $\mathbb{I}\{\theta_1^{(\cdot)} \leq x_1, \theta_2^{(\cdot)} \geq x_2\}$.

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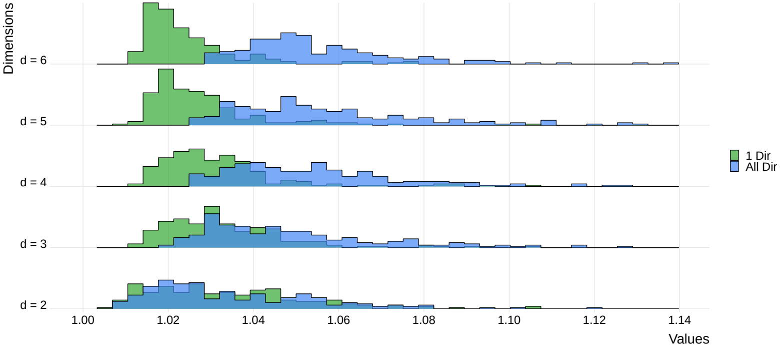

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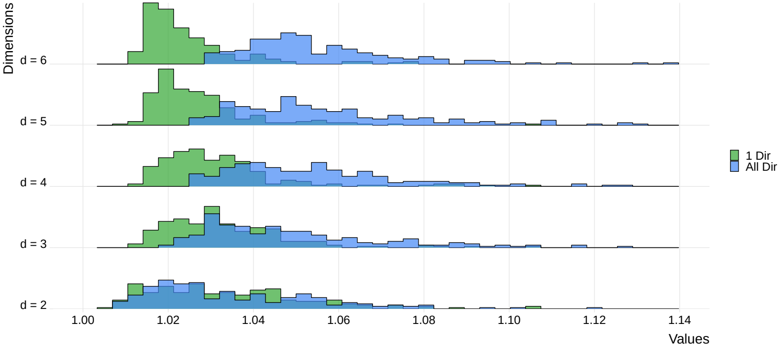

Alternative: computation of $\hat{R}_{\infty}$ for a univariate function of the parameters