Supplementary Material

Estimating quantiles in imperfect simulation models using conditional density estimation

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Proof of Lemma 3. Partition $[-\gamma_n, \gamma_n]^d$ into

$$N = \left(\left\lceil \frac{2 \cdot \gamma_n}{H_n/\sqrt{d}} \right\rceil \right)^d \leq \left(\frac{4 \cdot \sqrt{d} \cdot \gamma_n}{H_n} \right)^d$$

many cubes $A_1, \dots, A_N$ of side length at most $H_n/\sqrt{d}$. Let x_i be the center of A_i. Then $A_i \subseteq S_{H_n/2}(x_i)$ and $x \in S_{H_n/2}(x_i)$ implies $S_{H_n}(x) \supseteq S_{H_n/2}(x_i)$. Consequently we have

$$\int_{[-\gamma_n,\gamma_n]^d} \frac{1}{n \cdot \mathbf{P}_X(S_{H_n}(x))} \mathbf{P}_X(dx) \leq \sum_{i=1}^N \int_{S_{H_n/2}(x_i)} \frac{1}{n \cdot \mathbf{P}_X(S_{H_n}(x))} \mathbf{P}_X(dx)$$
$$\leq \sum_{i=1}^N \int_{S_{H_n/2}(x_i)} \frac{1}{n \cdot \mathbf{P}_X(S_{H_n/2}(x_i))} \mathbf{P}_X(dx) \leq \frac{N}{n},$$

which implies the assertion. □

Proof of Remark 4.

In what follows we show how to choose bandwidths h_n and H_n in order to minimize the expression (14). Here we ignore constants and logarithmic factors, so the aim is to minimize

$$\sqrt{\frac{A_n}{n \cdot H_n^d \cdot h_n}} + \frac{1}{n \cdot H_n^d} + A_n \cdot (C_1 \cdot H_n^r + C_2 \cdot h_n^s) \quad (37)$$

with respect to $h_n > 0$ and $H_n > 0$, where we have used the abbreviation

$$A_n = \int_{[-\log(n),\log(n)]^d} |b_n(x) - a_n(x)| \, \mathbf{P}_X(dx).$$

If (h_n, H_n) minimizes (37), then h_n satisfies

$$\sqrt{\frac{A_n}{n \cdot H_n^d \cdot h_n}} = A_n \cdot C_2 \cdot h_n^s.$$

The last equation is equivalent to

$$\frac{1}{C_2^2 \cdot A_n \cdot n \cdot H_n^d} = h_n^{2s+1},$$

from which we conclude

$$h_n = C_2^{-2/(2s+1)} \cdot A_n^{-1/(2s+1)} \cdot n^{-1/(2s+1)} \cdot H_n^{-d/(2s+1)}.$$

Plugging that bandwidth back into (37) yields

$$\begin{aligned} &\frac{1}{n \cdot H_n^d} + A_n \cdot C_1 \cdot H_n^r + 2 \cdot A_n \cdot C_2 \cdot h_n^s \\ &= \frac{1}{n \cdot H_n^d} + A_n \cdot C_1 \cdot H_n^r + 2 \cdot C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)}. \end{aligned} \tag{38}$$

So the optimal $H_n > 0$ minimizes (38), and it is easy to see, that a value $H_n > 0$ which minimizes (38) does indeed exist.

The optimal $H_n > 0$ minimizing (38) must satisfy

$$\frac{-d}{n} \cdot H_n^{-d-1} + r \cdot A_n \cdot C_1 \cdot H_n^{r-1} - \frac{d \cdot s}{2s+1} \cdot 2 \cdot C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-1-d \cdot s/(2s+1)} = 0,$$

which we can rewrite as

$$\frac{d}{n} \cdot H_n^{-d} + \frac{d \cdot s}{2s+1} \cdot 2 \cdot C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)} - r \cdot A_n \cdot C_1 \cdot H_n^r = 0 \tag{39}$$

For the optimal H_n, either the first term on the left–hand side of (39) will be larger than the second one, or not. In the first case the optimal H_n lies between the solutions of

$$\frac{d}{n} \cdot H_n^{-d} = r \cdot A_n \cdot C_1 \cdot H_n^r$$

and of

$$2 \cdot \frac{d}{n} \cdot H_n^{-d} = r \cdot A_n \cdot C_1 \cdot H_n^r,$$

and in the second case it lies between the solutions of

$$\frac{d \cdot s}{2s+1} \cdot 2 \cdot C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)} = r \cdot A_n \cdot C_1 \cdot H_n^r$$

and

$$2 \cdot \frac{d \cdot s}{2s+1} \cdot 2 \cdot C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)} = r \cdot A_n \cdot C_1 \cdot H_n^r.$$

If we ignore again all constants we get that the optimal $H_n > 0$ either satisfies

$$\frac{1}{n \cdot H_n^d} = A_n \cdot C_1 \cdot H_n^r$$

or

$$C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)} = A_n \cdot C_1 \cdot H_n^r.$$

In the first case we get

$$H_n^{r+d} = A_n^{-1} \cdot C_1^{-1} \cdot n^{-1},$$

which implies

$$H_n = A_n^{-1/(r+d)} \cdot C_1^{-1/(r+d)} \cdot n^{-1/(r+d)}, \tag{40}$$

and in the second case we get

$$H_n^{(r \cdot (2s+1)+d \cdot s)/(2s+1)} = C_1^{-1} \cdot A_n^{-s/(2s+1)} \cdot C_2^{1/(2s+1)} \cdot n^{-s/(2s+1)},$$

from which we get

$$H_n = C_1^{-\frac{2s+1}{r \cdot (2s+1)+d \cdot s}} \cdot C_2^{\frac{1}{r \cdot (2s+1)+d \cdot s}} \cdot A_n^{-\frac{s}{r \cdot (2s+1)+d \cdot s}} \cdot n^{-\frac{s}{r \cdot (2s+1)+d \cdot s}}. \tag{41}$$

Plugging (40) into (38) and ignoring again all constants yields as an upper bound on the error

$$\begin{aligned} & A_n \cdot C_1 \cdot H_n^r + C_2^{1/(2s+1)} \cdot A_n^{(s+1)/(2s+1)} \cdot n^{-s/(2s+1)} \cdot H_n^{-d \cdot s/(2s+1)} \\ & = C_1^{\frac{d}{r+d}} \cdot A_n^{\frac{d}{r+d}} \cdot n^{-\frac{r}{r+d}} + C_1^{\frac{ds}{(r+d)(2s+1)}} \cdot C_2^{\frac{1}{2s+1}} A_n^{\frac{(r+d)(s+1)+ds}{(r+d)(2s+1)}} \cdot n^{-\frac{rs}{(r+d)(2s+1)}}. \end{aligned} \tag{42}$$

And plugging (41) into (38) and ignoring again all constants yields as an upper bound on the error

$$\begin{aligned} & \frac{1}{n \cdot H_n^d} + A_n \cdot C_1 \cdot H_n^r \\ & = C_1^{\frac{(2s+1)d}{r(2s+1)+ds}} \cdot C_2^{-\frac{d}{r(2s+1)+ds}} \cdot A_n^{\frac{ds}{r(2s+1)+ds}} \cdot n^{-\frac{r(2s+1)}{r(2s+1)+ds}} \\ & \quad + C_1^{\frac{ds}{r(2s+1)+ds}} \cdot C_2^{\frac{r}{r(2s+1)+ds}} \cdot A_n^{\frac{r(s+1)+ds}{r(2s+1)+ds}} \cdot n^{-\frac{rs}{r(2s+1)+ds}}. \end{aligned} \tag{43}$$

From this we can conclude that (up to a logarithmic factor) the minimal value of (14) is given by the minimum of (42) and (43).