Supplementary Material

Estimation of an improved surrogate model in uncertainty quantification by neural networks

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January 23, 2020

Proof of Theorem 2. *In the first step of the proof* we show that we can assume w.l.o.g.

$$\bar{Y}_{i,n} \in [-\beta_n, \beta_n] \quad \text{for all} \quad i = 1, \dots, n + L_n. \tag{43}$$

To do this, we let

$$A_n = \left\{ |\bar{Y}_{i,n}| \leq \beta_n \quad \text{for all } i = 1, \dots, n + L_n \right\}$$

be the event that all $\bar{Y}_{i,n}$ be bounded in absolutely value by β_n. The union bound together with Markov inequality and (32) implies

$$\begin{aligned} \mathbf{P}(A_n^c) &\leq (n + L_n) \cdot \max_{i=1,\dots,n+L_n} \mathbf{P}\{|\bar{Y}_{i,n}| > \beta_n\} \leq (n + L_n) \cdot \frac{\max_{i=1,\dots,n+L_n} \mathbf{E}\left\{|\bar{Y}_{i,n}|^3\right\}}{\beta_n^3} \\ &\leq \frac{c_{69}}{n}. \end{aligned}$$

On the event A_n the estimate m_n coincides with the estimate $m_n^{(trunc)}$ defined by

$$\tilde{m}_n^{(trunc)}(\cdot) = \arg \min_{f \in \mathcal{F}_n} \left(\sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - T_{\beta_n} \bar{Y}_{i,n}|^2 + pen_n^2(f) \right)$$

and

$$m_n^{(trunc)}(x) = T_\beta \tilde{m}_n^{(trunc)}(x) \quad (x \in \mathbb{R}^d).$$

From this we can conclude that

$$\begin{aligned} &\mathbf{E} \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) \\ &\leq \mathbf{E} \left\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) \cdot I_{A_n} \right\} + 4 \cdot \beta^2 \cdot \mathbf{P}(A_n^c) \end{aligned}$$

$$= \mathbf{E}\left\{\int |m_n^{(trunc)}(x) - m(x)|^2 \mathbf{P}_X(dx) \cdot I_{A_n}\right\} + 4 \cdot \beta^2 \cdot \mathbf{P}(A_n^c)$$
$$\leq \mathbf{E} \int |m_n^{(trunc)}(x) - m(x)|^2 \mathbf{P}_X(dx) + 4 \cdot \beta^2 \cdot \frac{c_{69}}{n},$$

which completes the first step of the proof.

So from now on we assume that (43) holds. Set

$$\gamma_n = w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}$$

and

$$T_n = \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) - \left(9 \cdot \inf_{f \in \mathcal{F}_n} \left(pen_n^2(f) + \sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2\right) + 384 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2\right).$$

In the second step of the proof we show that the assertion follows from

$$\int_{12 \cdot \gamma_n}^{4 \cdot \beta^2} \mathbf{P}\{T_n > t\}\, dt \leq \frac{c_{70}}{n} + c_{71} \cdot \left(w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}\right).$$

To do this, we observe

$$\mathbf{E} \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx)$$
$$\leq \mathbf{E}\Bigg\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) - \left(9 \cdot \inf_{f \in \mathcal{F}_n} \left(pen_n^2(f) + \sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2\right) + 384 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2\right)\Bigg\}$$
$$+ \mathbf{E}\left\{9 \cdot \inf_{f \in \mathcal{F}_n} \left(pen_n^2(f) + \sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2\right) + 384 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2\right\}$$
$$\leq 12 \cdot \gamma_n + \int_{12 \cdot \gamma_n}^{\infty} \mathbf{P}\{T_n > t\} dt + 384 \cdot \mathbf{E}\left\{\sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2\right\}$$
$$+ 9 \cdot \inf_{f \in \mathcal{F}_n} \left(pen_n^2(f) + \int |f(x) - m(x)|^2 \mathbf{P}_X(dx)\right)$$
$$= 12 \cdot \gamma_n + \int_{12 \cdot \gamma_n}^{4 \cdot \beta^2} \mathbf{P}\{T_n > t\} dt + 384 \cdot \mathbf{E}\left\{\sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2\right\}$$
$$+ 9 \cdot \inf_{f \in \mathcal{F}_n} \left(pen_n^2(f) + \int |f(x) - m(x)|^2 \mathbf{P}_X(dx)\right),$$

where the last equation holds since $T_n \leq 4\beta^2$. The definition of γ_n and of the weights implies the assertion of step 2.

In the third step of the proof we show that we have for $t > 0$

$$\mathbf{P}\{T_n > t\} \leq P_{1,n}(t) + P_{2,n}(t),$$

where

$$\begin{aligned} P_{1,n}(t) &= \mathbf{P}\Bigg\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) \\ &\qquad > \frac{t}{2} + 3 \cdot pen_n^2(\tilde{m}_n) + 3 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |m_n(X_i) - m(X_i)|^2 \Bigg\} \end{aligned}$$

and

$$\begin{aligned} P_{2,n}(t) &= \mathbf{P}\Bigg\{ 3 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |m_n(X_i) - m(X_i)|^2 + 3 \cdot pen_n^2(\tilde{m}_n) \\ &\qquad > \frac{t}{2} + 9 \cdot \inf_{f \in \mathcal{F}_n} \left(\sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2 + pen_n^2(f) \right) \\ &\qquad\qquad + 384 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2 \Bigg\}. \end{aligned}$$

Using

$$\begin{aligned} & T_n \\ &= \left(\int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) - 3 \cdot pen_n^2(\tilde{m}_n) - 3 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |m_n(X_i) - m(X_i)|^2 \right) \\ &\quad + \Bigg(3 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |m_n(X_i) - m(X_i)|^2 + 3 \cdot pen_n^2(\tilde{m}_n) \\ &\quad - \left(9 \cdot \inf_{f \in \mathcal{F}_n} \left(\sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2 + pen_n^2(f) \right) + 384 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2 \right) \Bigg) \\ &=: T_{1,n} + T_{2,n} \end{aligned}$$

this immediately follows from

$$\mathbf{P}\{T_n > t\} = \mathbf{P}\{T_{1,n} + T_{2,n} > t\} \leq \mathbf{P}\{T_{1,n} > t/2\} + \mathbf{P}\{T_{2,n} > t/2\}.$$

In the fourth step of the proof we derive a upper bound on

$$\int_{12 \cdot \gamma_n}^{4 \cdot \beta^2} P_{1,n}(t)\, dt.$$

Let $12 \cdot \gamma_n \leq t \leq 4 \cdot \beta^2$. The definition of the weights together with

$$a + b > c + d \quad \Rightarrow \quad (a > c \text{ or } b > d)$$

implies that we have

$$
\begin{aligned}
P_{1,n}(t) \quad \leq \quad & \mathbf{P}\Bigg\{ w^{(n)} \cdot \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) > \frac{w^{(n)} \cdot \delta_n}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{2} \\
& \qquad + w^{(n)} \cdot 3 \cdot pen_n^2(\tilde{m}_n) + w^{(n)} \cdot 3 \cdot \frac{1}{n} \cdot \sum_{i=1}^{n} |m_n(X_i) - m(X_i)|^2 \Bigg\} \\
& + \mathbf{P}\Bigg\{ (1 - w^{(n)}) \cdot \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) \\
& \quad > \frac{(1 - w^{(n)}) \cdot \delta_{L_n}}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{2} + (1 - w^{(n)}) \cdot 3 \cdot pen_n^2(\tilde{m}_n) \\
& \qquad + (1 - w^{(n)}) \cdot 3 \cdot \frac{1}{L_n} \cdot \sum_{i=n+1}^{n+L_n} |m_n(X_i) - m(X_i)|^2 \Bigg\} \\
& \leq \mathbf{P}\Bigg\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) > \frac{\delta_n}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{2} \\
& \qquad + 3 \cdot pen_n^2(\tilde{m}_n) + 3 \cdot \frac{1}{n} \cdot \sum_{i=1}^{n} |m_n(X_i) - m(X_i)|^2 \Bigg\} \\
& + \mathbf{P}\Bigg\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) > \frac{\delta_{L_n}}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{2} \\
& \qquad + 3 \cdot pen_n^2(\tilde{m}_n) + 3 \cdot \frac{1}{L_n} \cdot \sum_{i=n+1}^{n+L_n} |m_n(X_i) - m(X_i)|^2 \Bigg\} \\
& = P_{1,n}^{(1)}(t) + P_{1,n}^{(2)}(t).
\end{aligned}
$$

Set

$$
\bar{\delta}_n := \frac{\delta_n}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{12} \quad \text{and} \quad \bar{\delta}_{L_n} := \frac{\delta_{L_n}}{w^{(n)} \cdot \delta_n + (1 - w^{(n)}) \cdot \delta_{L_n}} \cdot \frac{t}{12}.
$$

We have

$$
\begin{aligned}
& P_{1,n}^{(1)}(t) \\
& = \mathbf{P}\left\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) > 6 \cdot \bar{\delta}_n + 3 \cdot pen_n^2(\tilde{m}_n) + 3 \frac{1}{n} \sum_{i=1}^{n} |m_n(X_i) - m(X_i)|^2 \right\} \\
& \leq \mathbf{P}\left\{ \int |m_n(x) - m(x)|^2 \mathbf{P}_X(dx) > \bar{\delta}_n + 3 \cdot pen_n^2(\tilde{m}_n) + 3 \frac{1}{n} \sum_{i=1}^{n} |m_n(X_i) - m(X_i)|^2 \right\}.
\end{aligned}
$$

Next we want to use Lemma 4 from Kohler and Krzyżak (2017b) on the above probability, where we replace β_n in the notation of Lemma 4 by β. The assumptions of the lemma are satisfied since (34) and (36) hold for every $k \geq n$. Thus

$$\mathbf{P}\left\{\int |m_n(x)-m(x)|^2\mathbf{P}_X(dx) > \bar{\delta}_n + 3\cdot pen_n^2(\tilde{m}_n) + 3\frac{1}{n}\sum_{i=1}^{n}|m_n(X_i)-m(X_i)|^2\right\}$$
$$\leq c_{72}\cdot\exp\left(-\frac{n\cdot\bar{\delta}_n}{c_{72}\cdot\beta^2}\right)$$

holds. For $P_{1,n}^{(2)}$ we use an analogous transformation, apply Lemma 4, use the sample size L_n instead of n and replace again β_n by β and obtain

$$\begin{aligned} P_{1,n}^{(2)} &\leq \mathbf{P}\Bigg\{\int |m_n(x)-m(x)|^2\mathbf{P}_X(dx) > \bar{\delta}_{L_n} + 3\cdot pen_n^2(\tilde{m}_n) \\ &\qquad\qquad + 3\frac{1}{L_n}\sum_{i=n+1}^{n+L_n}|m_n(X_i)-m(X_i)|^2\Bigg\}. \\ &\leq c_{72}\cdot\exp\left(-\frac{L_n\cdot\bar{\delta}_{L_n}}{c_{72}\cdot\beta^2}\right). \end{aligned}$$

The results for $P_{1,n}^{(1)}$ and $P_{1,n}^{(2)}$ are implying

$$\begin{aligned} \int_{12\cdot\gamma_n}^{4\cdot\beta^2} P_{1,n}(t)dt &\leq \frac{c_{73}\cdot\beta^2}{n}\cdot\frac{w^{(n)}\cdot\delta_n+(1-w^{(n)})\cdot\delta_{L_n}}{\delta_n}\cdot\exp\left(-\frac{n}{c_{73}\cdot\beta^2}\cdot\delta_n\right) \\ &\quad +\frac{c_{73}\cdot\beta^2}{L_n}\cdot\frac{w^{(n)}\cdot\delta_n+(1-w^{(n)})\cdot\delta_{L_n}}{\delta_{L_n}}\cdot\exp\left(-\frac{L_n}{c_{73}\cdot\beta^2}\cdot\delta_{L_n}\right) \\ &\leq \frac{c_{73}}{n}\cdot\frac{\delta_n}{\delta_n}\cdot\exp\left(-\frac{c_{22}\cdot\beta^2}{c_{73}\cdot\beta^2}\right) \\ &\quad +\frac{c_{73}\cdot\beta^2\cdot\left(w^{(n)}\cdot\delta_n+(1-w^{(n)})\cdot\delta_{L_n}\right)}{c_{22}\cdot\beta^2}\cdot\exp\left(-\frac{c_{22}\cdot\beta^2}{c_{73}\cdot\beta^2}\right) \\ &\leq \frac{c_{74}}{n}+c_{75}\cdot\left(w^{(n)}\cdot\delta_n+(1-w^{(n)})\cdot\delta_{L_n}\right) \end{aligned}$$

where we have used $\delta_n \geq \delta_{L_n} > 0$, and that (34) implies

$$\delta_n\cdot n > c_{22}\cdot\beta^2 \quad\text{and}\quad \delta_{L_n}\cdot L_n > c_{22}\cdot\beta^2.$$

In the fifth step of the proof we derive a upper bound on

$$\int_{12\cdot\gamma_n}^{4\cdot\beta^2} P_{2,n}(t)\,dt.$$

Since $|m(x)| \leq \beta \leq \beta_n$ ($x \in \mathbb{R}^d$) and $w_i \geq 0$ ($i \in \{1,\ldots,n+L_n\}$) we have

$$\sum_{i=1}^{n+L_n} w_i\cdot|m_n(X_i)-m(X_i)|^2 \leq \sum_{i=1}^{n+L_n} w_i\cdot|T_{\beta_n}\tilde{m}_n(X_i)-m(X_i)|^2$$

which implies

$$
\begin{aligned}
P_{2,n}(t) \quad \leq \quad \mathbf{P}\Bigg\{ & \sum_{i=1}^{n+L_n} w_i \cdot |T_{\beta_n}\tilde{m}_n(X_i) - m(X_i)|^2 + pen_n^2(\tilde{m}_n) \\
& > \frac{t}{6} + 3 \cdot \inf_{f \in \mathcal{F}_n} \left(\sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2 + pen_n^2(f) \right) \\
& \quad + 128 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2 \Bigg\}.
\end{aligned}
$$

Choose $m_n^* \in \mathcal{F}_n$ such that

$$
\begin{aligned}
& 3 \cdot \left(\sum_{i=1}^{n+L_n} w_i \cdot |m_n^*(X_i) - m(X_i)|^2 + pen_n^2(m_n^*) \right) \\
& \leq 3 \cdot \inf_{f \in \mathcal{F}_n} \left(\sum_{i=1}^{n+L_n} w_i \cdot |f(X_i) - m(X_i)|^2 + pen_n^2(f) \right) + \frac{t}{12}
\end{aligned}
$$

Then we can conclude by Lemma 1 from Kohler and Krzyżak (2017b) that the above probability is bounded by

$$
\begin{aligned}
& \mathbf{P}\Bigg\{ \sum_{i=1}^{n+L_n} w_i \cdot |T_{\beta_n}\tilde{m}_n(X_i) - m(X_i)|^2 + pen_n^2(\tilde{m}_n) \\
& \qquad \geq \frac{t}{12} + 3 \cdot \left(\sum_{i=1}^{n+L_n} w_i \cdot |m_n^*(X_i) - m(X_i)|^2 + pen_n^2(m_n^*) \right) + 128 \cdot \sum_{i=1}^{n+L_n} w_i \cdot |Y_i - \bar{Y}_{i,n}|^2 \Bigg\} \\
& \leq \mathbf{P}\Bigg\{ \sum_{i=1}^{n+L_n} w_i \cdot (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
& \qquad \geq \frac{1}{24} \cdot \left(\sum_{i=1}^{n+L_n} w_i \cdot |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + \frac{t}{72} \Bigg\}
\end{aligned}
$$

The definition of the weights together with

$$
a + b > c + d \quad \Rightarrow \quad (a > c \text{ or } b > d)
$$

implies

$$
\begin{aligned}
& \mathbf{P}\Bigg\{ \sum_{i=1}^{n+L_n} w_i \cdot (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
& \qquad \geq \frac{1}{24} \cdot \left(\sum_{i=1}^{n+L_n} w_i \cdot |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + \frac{t}{72} \Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
&\leq \mathbf{P}\Bigg\{ \frac{w^{(n)}}{n} \sum_{i=1}^{n} (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
&\qquad \geq \frac{w^{(n)}}{24} \cdot \left(\frac{1}{n} \sum_{i=1}^{n} |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + w^{(n)} \cdot \frac{\bar{\delta}_n}{6} \Bigg\} \\
&\quad + \mathbf{P}\Bigg\{ \frac{(1-w^{(n)})}{L_n} \sum_{i=n+1}^{n+L_n} (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
&\qquad \geq \frac{(1-w^{(n)})}{24} \cdot \left(\frac{1}{L_n} \sum_{i=n+1}^{n+L_n} |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + (1-w^{(n)}) \cdot \frac{\bar{\delta}_{L_n}}{6} \Bigg\} \\
&\leq \mathbf{P}\Bigg\{ \frac{1}{n} \sum_{i=1}^{n} (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
&\qquad \geq \frac{1}{24} \cdot \left(\frac{1}{n} \sum_{i=1}^{n} |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + \frac{1}{6} \cdot \bar{\delta}_n \Bigg\} \\
&\quad + \mathbf{P}\Bigg\{ \frac{1}{L_n} \sum_{i=n+1}^{n+L_n} (T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)) \cdot (Y_i - m(X_i)) \\
&\qquad \geq \frac{1}{24} \cdot \left(\frac{1}{L_n} \sum_{i=n+1}^{n+L_n} |T_{\beta_n}\tilde{m}_n(X_i) - m_n^*(X_i)|^2 + pen_n^2(\tilde{m}_n) \right) + \frac{1}{6} \cdot \bar{\delta}_{L_n} \Bigg\} \\
&= P_{2,n}^{(1)}(t) + P_{2,n}^{(2)}(t).
\end{aligned}
$$

Next we want to use Lemma 3 from Kohler and Krzyżak (2017b) in order to bound $P_{2,n}^{(1)}(t)$. The assumptions of the Lemma are satisfied since (34) and (35) hold for every $k \geq n$. Thus

$$P_{2,n}^{(1)}(t) \leq c_{76} \cdot \exp\left(-\frac{n \cdot \min\{\bar{\delta}_n, \sigma_0^2\}}{c_{76}} \right)$$

and because of $t \leq 4\beta^2$ we can w.l.o.g. assume that $\sigma_0^2 \geq \bar{\delta}_n$ holds. Thus

$$P_{2,n}^{(1)}(t) \leq c_{76} \exp\left(-\frac{n\bar{\delta}_n}{c_{76}} \right)$$

and by the same arguments we can apply Lemma 3 from Kohler and Krzyżak (2017) and obtain

$$P_{2,n}^{(2)}(t) \leq c_{77} \exp\left(-\frac{L_n\bar{\delta}_{L_n}}{c_{77}} \right).$$

Analogously as before $\delta_n \geq \delta_{L_n} > 0$ and

$$\delta_n \cdot n > c_{22} \quad \text{and} \quad \delta_{L_n} \cdot L_n > c_{22}$$

implies

$$\int_{12\cdot\gamma_n}^{4\cdot\beta^2} P_{2,n}(t)dt \leq \frac{c_{78}}{n} + c_{79} \cdot \left(w^{(n)} \cdot \delta_n + (1-w^{(n)}) \cdot \delta_{L_n} \right).$$

Summarizing the above results we get the assertion. □