Supplementary Material

Kernel-based sensitivity indices for any model behavior and screening

A: Proof of Proposition 1

Knowing that the density of **X** is given by $\rho(\mathrm{x}) = c\left(F_1(x_1), \dots, F_d(x_d)\right)\prod_{j=1}^{d} \rho_j(x_j)$, we can write thanks to Equation (3)

$$\rho^w(\mathbf{x}) = \frac{w(\mathbf{x})}{\mathbb{E}_F[w(\mathbf{X})]} c\left(F_1(x_1), \dots, F_d(x_d)\right) \prod_{j=1}^{d} \rho_j(x_j).$$

B: Proof of Theorem 1

The following proof is simpler than the general one provided in Lamboni (2023). Since $\rho^w(\mathbf{x}) = \frac{w_e(\mathbf{x})}{\mathbb{E}_{F_{ind}}[w_e(\mathbf{Y})]} \prod_{j=1}^{d} \rho_j(x_j)$ (see Proposition 1), the density of $\mathbf{X}_{\sim u}^w \mid \mathbf{X}_u^w$ becomes

$$\rho_{\sim u|u}^w(\mathbf{x}_{\sim u} \mid \mathbf{x}_u^w) = \frac{w_e(\mathbf{x}_u^w, \mathbf{x}_{\sim u})}{\mathbb{E}_{F_{\text{ind}}}[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})]} \prod_{j \in (\sim u)} \rho_j(x_j),$$

and we can write (bearing in mind $(\sim u) = (\pi_1, \dots, \pi_{|\pi|})$)

$$F_{\sim u|u}^w(\mathbf{x}_{\sim u} \mid \mathbf{x}_u^w) == \mathbb{E}_{F_{ind}}\left[\frac{w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})}{\mathbb{E}_{F_{ind}}[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})]} \prod_{j=1}^{|\pi|} \mathbb{1}_{\left[-\infty, x_{\pi_j}\right]}\left(Y_{\pi_j}\right)\right].$$

Knowing that $X_{\pi_j} \stackrel{d}{=} F_{\pi_j}^{-1}\left(U_{\pi_j}\right)$ with $U_{\pi_j} \sim \mathcal{U}(0,1)$ and using the theorem of transfer, we have

$$F_{\sim u|u}^w(\mathbf{x}_{\sim u} \mid \mathbf{x}_u^w) = \mathbb{E}_{\mathbf{U}_\pi}\left[\frac{w_e\left(\mathbf{x}_u^w, F_{\pi_1}^{-1}(U_{\pi_1}), \dots, F_{\pi_{|\pi|}}^{-1}\left(U_{\pi_{|\pi|}}\right)\right)}{\mathbb{E}_{F_{ind}}[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})]} \prod_{j=1}^{|\pi|} \mathbb{1}_{\left[-\infty, x_{\pi_j}\right]}\left(F_{\pi_j}^{-1}\left(U_{\pi_j}\right)\right)\right],$$

with $\mathbf{U}_\pi := \left(U_{\pi_j}, j = 1, \dots, |\pi|\right) \sim \mathcal{U}(0,1)^d$. As F_j is strictly increasing, we have

$$\begin{aligned} F_{\sim u|u}^w(\mathbf{x}_{\sim u} \mid \mathbf{x}_u^w) \quad &= \mathbb{E}_{\mathbf{U}_\pi}\left[\frac{w_e\left(\mathbf{x}_u^w, F_{\pi_1}^{-1}(U_{\pi_1}), \dots, F_{\pi_{|\pi|}}^{-1}\left(U_{\pi_{|\pi|}}\right)\right)}{\mathbb{E}_{F_{ind}}[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})]} \prod_{j=1}^{|\pi|} \mathbb{1}_{\left[0, F_{\pi_j}(x_{\pi_j})\right]}\left(U_{\pi_j}\right)\right] \\ &= \int_0^{F_{\pi_1}(x_{\pi_1})} \dots \int_0^{F_{\pi_{|\pi|}}(x_{\pi_{|\pi|}})} \frac{w_e\left(\mathbf{x}_u^w, F_{\pi_1}^{-1}(v_{\pi_1}), \dots, F_{\pi_{|\pi|}}^{-1}\left(v_{\pi_{|\pi|}}\right)\right)}{\mathbb{E}_{F_{ind}}[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})]} \prod_{j=1}^{|\pi|} dv_{\pi_j}. \end{aligned}$$

Now, if we use $\mathbf{V}_\pi := \left(V_{\pi_k} \sim \mathcal{U}\left(0, u_{\pi_k}\right), k = 1, \dots, |\pi|\right)$ for a random vector of independent variables and

$$
\begin{aligned}
W(\mathbf{u}_\pi;\mathbf{x}_u^w) \quad &:= \int_0^{u_{\pi_1}} \dots \int_0^{u_{\pi_{|\pi|}}} \frac{w_e\left(\mathbf{x}_u^w, F_{\pi_1}^{-1}(v_{\pi_1}), \dots, F_{\pi_{|\pi|}}^{-1}\left(v_{\pi_{|\pi|}}\right)\right)}{\mathbb{E}_{F_{ind}}\left[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})\right]} \prod_{j=1}^{|\pi|} dv_{\pi_j} \\
&= \frac{\mathbb{E}_{\mathbf{V}_\pi}\left[w_e\left(\mathbf{x}_u^w, F_{\pi_1}^{-1}(V_{\pi_1}), \dots, F_{\pi_{|\pi|}}^{-1}\left(V_{\pi_{|\pi|}}\right)\right)\right]}{\mathbb{E}_{F_{ind}}\left[w_e(\mathbf{x}_u^w, \mathbf{Y}_{\sim u})\right]} \prod_{j=1}^{|\pi|} u_{\pi_j},
\end{aligned}
$$

then W is a CDF of a random vector having $(0,1)^{d-|u|}$ as the support, and we have

$$
F_{\sim u|u}^w(\mathbf{x}_{\sim u} \mid \mathbf{x}_u^w) = W\left(F_{\pi_1}(x_{\pi_1}), \dots, F_{\pi_{|\pi|}}\left(x_{\pi_{|\pi|}}\right); \mathbf{x}_u^w\right).
$$

C: Proof of Lemma 1

Since $\mathbf{X}_u^w, \mathbf{X}_u^{w'}$ are i.i.d. and $\Theta = \{\theta_0\}$, we can write thanks to Proposition 2

$$
\begin{aligned}
f_u^{fo}(\mathbf{X}_u^w) \quad &= \mathbb{E}_U\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right)\right] - \frac{\mathbb{E}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U})\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]} \\
&= \mathbb{E}_U\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - \frac{\mathbb{E}_{\mathbf{Y}}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U})\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]}\right] \\
&= \mathbb{E}_U\left[f_u^{tot}(\mathbf{X}_u^w, \mathbf{U})\right].
\end{aligned}
$$

Using the convexity of ϕ and the definition of the kernel, the Jensen inequality yields

$$
\mathbb{E}\left[k\left(f_u^{fo}(\mathbf{X}_u^w), f_u^{fo}\left(\mathbf{X}_u^{w'}\right)\right)\right] \leq \mathbb{E}\left[k\left(f_u^{tot}(\mathbf{X}_u^w, \mathbf{U}), f_u^{tot}\left(\mathbf{X}_u^{w'}, \mathbf{U}'\right)\right)\right].
$$

Now, we are going to show that the total index is less than one. Let us consider the Dirac probability measure $\delta_{\mathbf{U}}(\mathbf{U}') := \delta_{\mathbf{0}}(\mathbf{U}' - \mathbf{U})$ and the zero-mean expression of the outputs $f_u^c(\mathbf{X}_u^w, \mathbf{U}) = \mathbb{E}\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - \frac{\mathbb{E}_{\mathbf{Y}}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U}')\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]} \mid \mathbf{U}, \mathbf{X}_u^w\right]$. We can then write

$$
\begin{aligned}
&\mathbb{E}\left[f_u^c(\mathbf{X}_u^w, \mathbf{U}) \mid \delta_{\mathbf{U}}(\mathbf{U}'), \mathbf{U}, \mathbf{X}_u^w\right] \\
= \quad &\mathbb{E}\left[\mathbb{E}\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - \frac{\mathbb{E}_{\mathbf{Y}}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U}')\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]} \mid \mathbf{U}, \mathbf{X}_u^w\right] \mid \delta_{\mathbf{U}}(\mathbf{U}'), \mathbf{U}, \mathbf{X}_u^w\right] \\
= \quad &\mathbb{E}\left[\mathbb{E}\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - \frac{\mathbb{E}_{\mathbf{Y}}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U}')\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]} \mid \delta_{\mathbf{U}}(\mathbf{U}'), \mathbf{U}, \mathbf{X}_u^w\right] \mid \mathbf{U}, \mathbf{X}_u^w\right] \\
= \quad &\mathbb{E}\left[f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - \frac{\mathbb{E}_{\mathbf{Y}}\left[f\left(\mathbf{Y}_u, r(\mathbf{Y}_u, \mathbf{U})\right)w_e(\mathbf{Y})\right]}{\mathbb{E}[w_e(\mathbf{Y})]} \mid \mathbf{U}, \mathbf{X}_u^w\right] = f_u^{tot}(\mathbf{X}_u^w, \mathbf{U}),
\end{aligned}
$$

bearing in mind the formal definition of conditional expectation. The second result holds by applying the conditional Jensen inequality.

For the upper bound of the total index, knowing that $f_u^*\left(\mathbf{X}_u^w, \mathbf{X}_u^{w'}, \mathbf{U}\right) = f\left(\mathbf{X}_u^w, r(\mathbf{X}_u^w, \mathbf{U})\right) - f\left(\mathbf{X}_u^{w'}, r\left(\mathbf{X}_u^{w'}, \mathbf{U}\right)\right)$, we can write $f_u^{\text{tot}}(\mathbf{X}_u^w, \mathbf{U}) = \mathbb{E}_{\mathbf{X}_u^{w'}}\left[f_u^*\left(\mathbf{X}_u^w, \mathbf{X}_u^{w'}, \mathbf{U}\right)\right]$, and the result follows.

D: Proof of Theorem 2

First, the consistency of the estimators holds by applying the Slutsky theorem bearing in mind the Taylor expansion, that is,

$$k\left(\widehat{f_u^{fo}}(\mathbf{Y}_{i,u}), \widehat{f_u^{fo}}(\mathbf{Y}'_{i,u})\right) = k\left(f_u^{fo}(\mathbf{Y}_{i,u}), f_u^{fo}(\mathbf{Y}'_{i,u})\right)$$
$$+\nabla^T k\left(f_u^{fo}(\mathbf{Y}_u), f_u^{fo}(\mathbf{Y}'_u)\right)\begin{bmatrix}\widehat{f_u^{fo}}(\mathbf{Y}_{i,u}) - f_u^{fo}(\mathbf{Y}_{i,u}) \\ \widehat{f_u^{fo}}(\mathbf{Y}'_{i,u}) - f_u^{fo}(\mathbf{Y}'_{i,u})\end{bmatrix} + R_{m_1},$$

with $R_{m_1} \xrightarrow{P} 0$ when $m_1 \to \infty$. We obtain the results by applying the law of large numbers Second, the central limit theorem ensures that

$$\sqrt{m}\left(\frac{1}{m}\sum_{i=1}^{m} k\left(\widehat{f_u^{fo}}(\mathbf{Y}_{i,u}), \widehat{f_u^{fo}}(\mathbf{Y}'_{i,u})\right) w_e(\mathbf{Y}_i) w_e(\mathbf{Y}'_i) - D_u^k\right) \xrightarrow{D} \mathcal{N}\left(0, \sigma_u^{fo}\right),$$

with $D_u^k = \mathbb{E}\left[k\left(f_u^{fo}(\mathbf{Y}_u), f_u^{fo}(\mathbf{Y}'_u)\right) w_e(\mathbf{Y}) w_e(\mathbf{Y}')\right]$.

Third, the asymptotic distributions are straightforward using the Slutsky theorem under the technical assumption $m/M \to 0,\ m_1/M \to 0$ (see Lamboni (2020b, 2019) for more details).

E: Derivation of SFs used in Section 5.1

Using the model output and the dependency models, we can write

$$\begin{aligned} f_1^{fo}(X_1^w) &= (X_1^w)^2(1 - \mathbb{E}[Z_2] - \mathbb{E}[Z_3(1 - Z_2)]) - \mathbb{E}[(X_1^w)^2](1 - \mathbb{E}[Z_2] - \mathbb{E}[Z_3(1 - Z_2)]) \\ &= \left[(X_1^w)^2 - \mathbb{E}[(X_1^w)^2]\right](1 - \mathbb{E}[Z_2] - \mathbb{E}[Z_3(1 - Z_2)]) \\ &= [(X_1^w)^2 - c/5](1 - 1/4 - 1/3(1 - 1/4)]) = \frac{1}{2}[(X_1^w)^2 - c/5]; \\ f_1^{tot}(X_1^w, Z_2, Z_3) &= \left[(X_1^w)^2 - \mathbb{E}[(X_1^w)^2]\right]\left(1 - Z_2 - Z_3(1 - Z_2)\right) = [(X_1^w)^2 - c/5]\left(1 - Z_2 - Z_3(1 - Z_2)\right). \end{aligned}$$

We also have

$$f^c(X_1^w, Z_2, Z_3) = f(\mathrm{X}^w) - c/10 - c/4 - c/4 = (X_1^w)^2\left(1 - Z_2 - Z_3(1 - Z_2)\right) + cZ_2 + cZ_3(1 - Z_2) - \frac{3}{5}c.$$

$$f^*\left(X_1^w, X_1^{w\prime}, Z_2, Z_3\right) = \left[(X_1^w)^2 - \left(X_1^{w\prime}\right)^2\right]\left(1 - Z_2 - Z_3(1 - Z_2)\right).$$