The solutions for the implementation exercises for this sheet can be found in the files *hw_sol_3_1_PDP_ICE_Interactions.R* and *hw_sol_3_4_ME.R* on Moodle.

**Solution 1:**

a) Derivation of PD function for $S = \{1\}$ (with $C = \{2\}$) given

$$\hat{f}(\mathbf{x}) = \hat{f}(x_1, x_2) = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_1 x_2 + \hat{\beta}_0$$

$$\begin{aligned}
f_{1,PD}(x_1) = \mathbb{E}_{x_2}\left(\hat{f}(x_1, x_2)\right) &= \int_{-\infty}^{\infty} \left(\hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_1 x_2 + \hat{\beta}_0\right) d\mathbb{P}(x_2) \\
&= \hat{\beta}_1 x_1 + \int_{-\infty}^{\infty} \hat{\beta}_2 x_2 + \hat{\beta}_3 x_1 x_2 \, d\mathbb{P}(x_2) + \hat{\beta}_0 \\
&= \hat{\beta}_1 x_1 + \int_{-\infty}^{\infty} (\hat{\beta}_2 + \hat{\beta}_3 x_1) x_2 \, d\mathbb{P}(x_2) + \hat{\beta}_0 \\
&= \hat{\beta}_1 x_1 + (\hat{\beta}_2 + \hat{\beta}_3 x_1) \cdot \int_{-\infty}^{\infty} x_2 \, d\mathbb{P}(x_2) + \hat{\beta}_0 \\
&= \hat{\beta}_1 x_1 + (\hat{\beta}_2 + \hat{\beta}_3 x_1) \cdot \mathbb{E}_{x_2}(x_2) + \hat{\beta}_0
\end{aligned}$$

b) PD function for $\hat{\beta}_0 = 0$, $\hat{\beta}_1 = -8$, $\hat{\beta}_2 = 0.2$, $\hat{\beta}_3 = 16$, $X_1 \sim Unif(-1, 1)$ and $X_2 \sim B(1, 0.5)$.

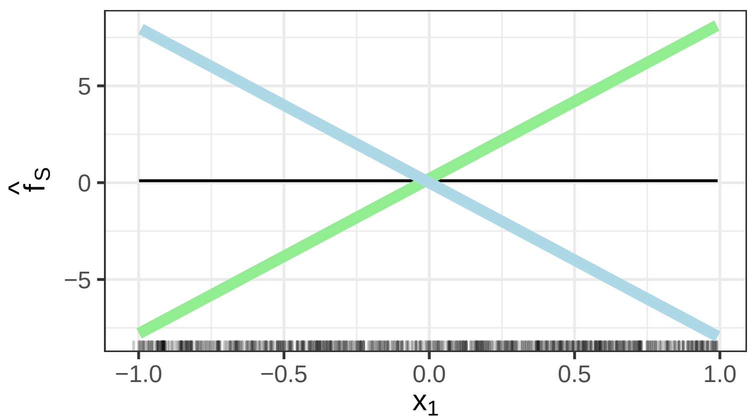
$$\begin{aligned}
f_{1,PD}(x_1) = \hat{\beta}_1 x_1 + (\hat{\beta}_2 + \hat{\beta}_3 x_1) \cdot \mathbb{E}_{x_2}(x_2) + \hat{\beta}_0 &= -8x_1 + (0.2 + 16x_1) \cdot \mathbb{E}_{x_2}(x_2) + 0 \\
&= -8x_1 + (0.2 + 16x_1) \cdot 0.5 \\
&= -8x_1 + 0.1 + 8x_1 \\
&= 0.1
\end{aligned}$$

c) ICE functions for group $X_2 = 1$ and for group $X_2 = 0$:

$$f_1(x_1) = \begin{cases} -8x_1 + (0.2 + 16x_1) \cdot 1 = 8x_1 + 0.2 & x_2 = 1 \\ -8x_1 + (0.2 + 16x_1) \cdot 0 = -8x_1 & x_2 = 0 \end{cases}$$

The light green dots correspond to group $X_2 = 1$, the light blue dots to group $X_2 = 0$.

d) The example illustrates that by the averaging of ICE curves for a PD plot we might obfuscate heterogeneous effects and interactions. Although the ICE curves here show a strong effect of $X_1$ on $Y$, the effect is not apparent in the PDP. Therefore, it is highly recommended to plot PD plots and ICE curves together.



e) , f) For the last two parts of the exercise, please find the solution in the file *hw_sol_3_1_PDP_ICE_Interactions.R*.

**Solution 2:**

The fitted model is

$$\hat{f}(x_1, x_2) = \theta_0 + \theta_1 x_1^2 + \theta_2 x_2^2 + \theta_{1,2} x_1 x_2, \quad (\theta_0, \theta_1, \theta_2, \theta_{1,2}) = (0,\ 1,\ 0.5,\ 2).$$

a) **Derivative marginal effect (dME)**

$$\mathrm{dME}_1(x_1, x_2) = \frac{\partial \hat{f}}{\partial x_1} = 2\theta_1 x_1 + \theta_{1,2} x_2 = 2x_1 + 2x_2.$$

*Discussion.* Because the model is quadratic in $x_1$, the derivative is a *linear* function of both $x_1$ and $x_2$. If the surface were exactly linear, this rate would coincide with any finite difference.

b) **Forward marginal effect (fME)** with step $h_1 > 0$

$$\mathrm{fME}_1(x_1, x_2; h_1) \ = \ \hat{f}(x_1 + h_1, x_2) - \hat{f}(x_1, x_2).$$

Expand $\hat{f}(x_1 + h_1, x_2)$:

$$\begin{aligned}\hat{f}(x_1+h_1, x_2) &= \theta_1 (x_1 + h_1)^2 + \theta_2 x_2^2 + \theta_{1,2}(x_1 + h_1) x_2 \\ &= \theta_1 \left[x_1^2 + 2x_1 h_1 + h_1^2\right] \ + \ \theta_2 x_2^2 \ + \ \theta_{1,2} x_1 x_2 + \theta_{1,2} h_1 x_2.\end{aligned}$$

Subtracting $\hat{f}(x_1, x_2)$ gives

$$\boxed{\mathrm{fME}_1(x_1, x_2; h_1) = 2\theta_1 x_1 h_1 + \theta_1 h_1^2 + \theta_{1,2} x_2 h_1} \ = \ 2x_1 h_1 + h_1^2 + 2x_2 h_1.$$

*Discussion.* The extra term $\theta_1 h_1^2$ captures curvature; it vanishes faster than linearly when $h_1 \to 0$, at which point fME converges to dME.

c) **Numerical evaluation at** $(x_1, x_2, h_1) = (1, 2, 1)$

$$\begin{aligned}\mathrm{dME}_1(1, 2) &= 2(1) + 2(2) = 6, \\ \mathrm{fME}_1(1, 2; 1) &= 2 \cdot 1 \cdot 1 + 1^2 + 2 \cdot 2 \cdot 1 = 2 + 1 + 4 = 7.\end{aligned}$$

*Why different?* The derivative 6 is the *instantaneous* slope. The finite step of 1 exposes curvature; the quadratic term makes the actual change go up to 7. Hence, using dME for a sizeable perturbation would misestimate (over- or under-predict) the effect.

d) **Non-Linearity Measure (NLM)** ($R^2$ of the linear secant along the path)

*Hints.*

- Compute $\mathrm{SSR} = \sum(\hat{f} - g)^2$ and $\mathrm{SST} = \sum(\hat{f} - \bar{f})^2$ from the table.
- Then evaluate $\mathrm{NLM} = 1 - \mathrm{SSR}/\mathrm{SST}$.
- Comment: Is the resulting NLM close enough to 1 to accept the secant as a faithful local explanation?

**Step 1: Path points.** For $T = 10$ equidistant $t_i \in [0, 1]$:

$$t_i = \frac{i}{9 + 1}, \quad x_1^{(i)} = 1 + t_i h_1 = 1 + 0.5\, t_i, \quad x_2^{(i)} = 2.$$

**Step 2: Model and secant values.**

$$f_i = \hat{f}(x_1^{(i)}, 2), \quad g_i = \hat{f}(1,2) + t_i \cdot \mathrm{fME}_1(1,2;0.5), \quad \hat{f}(1,2) = 7,\ \mathrm{fME} = 3.25.$$

**Step 3: Compute $R^2$.**

$$\mathrm{NLM} = 1 - \frac{\sum_{i=1}^{9}(f_i - g_i)^2}{\sum_{i=1}^{9}(f_i - \bar{f})^2}, \quad \bar{f} = \frac{1}{9}\sum f_i.$$

Numerically

$$\boxed{\mathrm{NLM}\ \approx\ 0.9967}.$$

*Interpretation.* Along the half-unit move in $x_1$, the quadratic surface is *almost* linear (NLM very close to 1). If we doubled $h_1$, the numerator would grow faster than the denominator, lowering NLM and signaling stronger curvature.

e) See the implementation in *hw_sol_3_4_ME.R*.