1. Notation List

- s, index of the feature of interest
- $\mathcal{X}_s$, feature of interest as a r.v.
- $\mathcal{X}_c = (\mathcal{X}_{/s},)$, the rest of the features in as a r.v.
- $\mathcal{X} = (\mathcal{X}_s, \mathcal{X}_c) = (\mathcal{X}_1, \cdots, \mathcal{X}_s, \cdots, \mathcal{X}_D)$, all input features as r.v.
- x_s, feature of interest
- $\mathbf{x}_c$, the rest of the features
- $\mathbf{x} = (x_s, \mathbf{x}_c) = (x_1, \cdots, x_s, \cdots, x_D)$, all the input features
- $\mathbf{X}$, design matrix/training set
- $f(\cdot) : \mathbb{R}^D \rightarrow \mathbb{R}$, black box function
- $f_s(\mathbf{x}) = \frac{\partial f(x_s, \mathbf{x}_c)}{\partial x_s}$, the partial derivative of the s-th feature
- D, dimensionality of the input
- N, number of training examples
- $\mathbf{x}^i$, i-th training example
- x_s^i, s-th feature of the i-th training example
- $\mathbf{x}_\mathbf{c}^i$, the rest of the features of the i-th training example
- $f_{\texttt{ALE}}(x_s) : \mathbb{R} \rightarrow \mathbb{R}$, ALE definition for the s-th feature
- $\hat{f}_{\texttt{DALE}}(x_s) : \mathbb{R} \rightarrow \mathbb{R}$, DALE approximation for the s-th feature
- $\hat{f}_{\texttt{ALE}}(x_s) : \mathbb{R} \rightarrow \mathbb{R}$, ALE approximation for the s-th feature
- z_{k-1}, z_k, the left and right limit of the k-th bin
- $\mathcal{S}_k = \{\mathbf{x}^i : x_s^i \in [z_{k-1}, z_k)\}$, the set of training points that belong to the k-th bin
- k_x the index of the bin that x belongs to
- $\hat{\mu}_k^s$, `DALE` approximation of the mean value inside a bin, equals $\frac{1}{|\mathcal{S}_k|} \sum_{i:x^i \in \mathcal{S}_k} f_s(\mathbf{x}^i)$
- $(\hat{\sigma}_k^s)^2$, `DALE` approximation of the variance inside a bin, equals $\frac{1}{|\mathcal{S}_k|-1} \sum_{i:x^i \in \mathcal{S}_k} (f_s(\mathbf{x}^i) - \hat{\mu}_k^s)^2$

2. Derivation of equations in the Background section

In this section, we present the derivations for obtaining the feature effect at the Background.

Example Definition.

The black-box function and the generating distribution are:

$$f(x_1, x_2) = \begin{cases} 1 - x_1 - x_2 & , \text{if } x_1 + x_2 \leq 1 \\ 0 & , \text{otherwise} \end{cases} \tag{1}$$

$$p(\mathcal{X}_1 = x_1, \mathcal{X}_2 = x_2) = \begin{cases} 1 & x_1 \in [0,1], x_2 = x_1 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

$$p(\mathcal{X}_1 = x_1) = \begin{cases} 1 & 0 \leq x_1 \leq 1 \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

$$p(\mathcal{X}_2 = x_2) = \begin{cases} 1 & 0 \leq x_2 \leq 1 \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

$$p(\mathcal{X}_2 = x_2 | \mathcal{X}_1 = x_1) = \delta(x_2 - x_1) \tag{5}$$

PDPlots.

The feature effect computed by PDP plots is:

$$\begin{aligned} f_{\texttt{PDP}}(x_1) = & \\ &= \mathbb{E}_{\mathcal{X}_2}[f(x_1, \mathcal{X}_2)] \\ &= \int_{x_2} f(x_1, x_2) p(x_2) \partial x_2 \\ &= \int_0^{1-x_1} (1 - x_1 - x_2) \partial x_2 + \int_{1-x_1}^1 0 \partial x_2 \\ &= \int_0^{1-x_1} 1 \partial x_2 + \int_0^{1-x_1} -x_1 \partial x_2 + \int_0^{1-x_1} -x_2 \partial x_2 \\ &= (1 - x_1) - x_1(1 - x_1) - \frac{(1 - x_1)^2}{2} \\ &= (1 - x_1)^2 - \frac{(1 - x_1)^2}{2} \\ &= \frac{(1 - x_1)^2}{2} \end{aligned} \tag{6}$$

Due to symmetry:

$$y = f_{\texttt{PDP}}(x_2) = \frac{(1 - x_2)^2}{2} \tag{7}$$

MPLOTS.

The feature effect computed by PDP plots is:

$$\begin{aligned}
f_{\texttt{MP}}(x_1) = & \\
& = \mathbb{E}_{\mathcal{X}_2|\mathcal{X}_1=x_1}[f(x_1, \mathcal{X}_2)] \\
& = \int_{x_2} f(x_1, x_2) p(x_2|x_1) \partial x_2 \\
& = f(x_1, x_1) = \\
& = \begin{cases} 1 - 2x_1, & x_1 \leq 0.5 \\ 0, & \text{otherwise} \end{cases}
\end{aligned} \tag{8}$$

Due to symmetry:

$$y = f_{\texttt{MP}}(x_2) = \begin{cases} 1 - 2x_2 & x_2 \leq 0.5 \\ 0, & \text{otherwise} \end{cases} \tag{9}$$

ALE

The feature effect computed by ALE is:

$$\begin{aligned}
f_{\texttt{ALE}}(x_1) = & \\
& = \int_{z_0}^{x_1} \mathbb{E}_{\mathcal{X}_2|\mathcal{X}_1=z} \left[\frac{\partial f}{\partial z}(z, \mathcal{X}_2) \right] \partial z \\
& = \int_{z_0}^{x_1} \int_{x_2} \frac{\partial f}{\partial z}(z, x_2) p(x_2|z) \partial x_2 \partial z = \\
& = \int_{z_0}^{x_1} \frac{\partial f}{\partial z}(z, z) \partial z = \\
& = \begin{cases} \int_{z_0}^{x_1} -1 \partial z & x_1 \leq 0.5 \\ \int_{z_0}^{0.5} -1 \partial z + \int_{.5}^{x_1} 0 \partial z & x_1 > 0.5 \end{cases} \\
& = \begin{cases} -x_1 & x_1 \leq 0.5 \\ -0.5 & x_1 > 0.5 \end{cases}
\end{aligned} \tag{10}$$

The normalization constant is:

$$\begin{aligned}
c & = -\mathbb{E}[\hat{f}_{ALE}(x_1)] \\
& = -\int_{-\infty}^{\infty} \hat{f}_{ALE}(x_1) \\
& = -\int_{0}^{0.5} -z \partial z - \int_{0.5}^{1} -0.5 \partial z \\
& = \frac{0.25}{2} + 0.25 = 0.375
\end{aligned} \tag{11}$$

Therefore, the normalized feature effect is:

$$y = f_{\texttt{ALE}}(x_1) = \begin{cases} 0.375 - x_1 & 0 \leq x_1 \leq 0.5 \\ -0.125 & 0.5 < x_1 \leq 1 \end{cases} \tag{12}$$

Due to symmetry:

$$y = f_{ALE}(x_2) = \begin{cases} 0.375 - x_2 & 0 \leq x_2 \leq 0.5 \\ -0.125 & 0.5 < x_2 \leq 1 \end{cases} \tag{13}$$

3. First-order and Second-order DALE approximation

In the main part of the paper, we presented the first order ALE approximation as

$$f_{\texttt{DALE}}(x_s) = \Delta x \sum_{k=1}^{k_x} \frac{1}{|\mathcal{S}_k|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} [f_s(\mathbf{x}^i)] \tag{14}$$

For keeping the equation compact, we ommit a small detail about the manipulation of the last bin. In reality, we take complete Δx steps until the $k_x - 1$ bin, i.e. the one that prepends the bin where x lies in. In the last bin, instead of a complete Δx step, we move only until the position x. Therefore, the exact first-order DALE approximation is

$$\begin{aligned} f_{\texttt{DALE}}(x_s) = \Delta x \sum_{k=1}^{k_x - 1} \frac{1}{|\mathcal{S}_k|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} [f_s(\mathbf{x}^i)] \\ + (x - z_{(k_x - 1)}) \frac{1}{|\mathcal{S}_{k_x}|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_{k_x}} [f_s(\mathbf{x}^i)] \end{aligned} \tag{15}$$

Following a similar line of thought we define the complete second-order DALE approximation as

$$\begin{aligned} f_{\texttt{DALE}}(x_l, x_m) = \Delta x_l \sum_{p=1}^{p_x - 1} \Delta x_m \sum_{q=1}^{q_x - 1} \frac{1}{|\mathcal{S}_{k,q}|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_{k,q}} f_{l,m}(\mathbf{x}^i) \\ + (x_l - z_{(p_x - 1)})(x_m - z_{(q_x - 1)}) \frac{1}{|\mathcal{S}_{p_x, q_x}|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_{p_x, q_x}} f_{l,m}(\mathbf{x}^i) \end{aligned} \tag{16}$$

4. Second-order ALE definition

The second-order ALE plot definintion is

$$f_{\texttt{ALE}}(x_l, x_m) = c + \int_{x_{l,min}}^{x_l} \int_{x_{m,min}}^{x_m} \mathbb{E}_{\mathcal{X}_c|X_l=z_l, X_m=z_m}[f_{l,m}(\mathbf{x})] \partial z_l \partial z_m \tag{17}$$

where $f_{l,m}(\mathbf{x}) = \frac{\partial^2 f(x)}{\partial x_l \partial x_m}$.

5. DALE variance inside each bin

In this section, we show that the variance of the local effect estimation inside a bin, i.e. $\mathrm{Var}[\hat{\mu}_k^s]$ equals with $\frac{(\sigma_k^s)^2}{|\mathcal{S}_k|}$, where $(\sigma_k^s)^2 = \mathrm{Var}[f_s(\mathbf{x})]$.

$$\begin{aligned}
\mathrm{Var}[\hat{\mu}_k^s] &= \mathrm{Var}[\frac{1}{|\mathcal{S}_k|} \sum_{i:x^i \in \mathcal{S}_k} f_s(\mathbf{x}^i)] \\
&= \frac{1}{|\mathcal{S}_k|^2} \sum_{i:x^i \in \mathcal{S}_k} \mathrm{Var}[f_s(\mathbf{x}^i)] \\
&= \frac{|\mathcal{S}_k|}{|\mathcal{S}_k|^2} \mathrm{Var}[f_s(\mathbf{x})] \\
&= \frac{(\sigma_k^s)^2}{|\mathcal{S}_k|}
\end{aligned} \tag{18}$$