



Regional effect plots for the interpretation of black box machine learning models

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Statistics Seminars 2023-2024 Department of Statistics, Athens University of Economics and Business 19/04/2024

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Feature Effect

Differential Accumulated Local Effects (DALE)

RHALE: Robust and Heterogeneity-aware Accumulated Local Effects

Regional effect plots - effector

Hypothetical (?) scenarios

• The computer vision subsystem of an autonomous vehicle leads the vehicle to take a left turn, in front of a car moving in the opposite direction¹

¹https:

^{//}www.theguardian.com/technology/2022/dec/22/tesla-crash-full-self-driving-mode-san-francisco ²https://www.technologyreview.com/2021/06/17/1026519/

racial-bias-noisy-data-credit-scores-mortgage-loans-fairness-machine-learning/

³https://www.propublica.org/article/machine-bias-risk-assessments-in-criminal-sentencing

Hypothetical (?) scenarios

- The computer vision subsystem of an autonomous vehicle leads the vehicle to take a left turn, in front of a car moving in the opposite direction¹
- The credit assessment system leads to the rejection of an application for a loan the client suspects racial bias²

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Hypothetical (?) scenarios

- The computer vision subsystem of an autonomous vehicle leads the vehicle to take a left turn, in front of a car moving in the opposite direction¹
- The credit assessment system leads to the rejection of an application for a loan the client suspects racial bias²
- A model that assesses the risk of future criminal offenses (and used for decisions on parole sentences) is biased against black prisoners³

¹https:

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Questions

- Why did a model make a specific decision?
- What could we change so that the model will make a different decision?
- Can we summarize and predict the model's behavior?

Today we focus on the last question

Taxonomy of interpretability methods

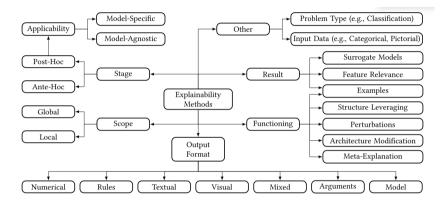


Figure: Timo Speith, "A Review of Taxonomies of Explainable Artificial Intelligence (XAI) Methods". In 2022 ACM Conference on Fairness, Accountability, and Transparency (FAccT '22), 2022 (Speith, 2022)

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Interpretable models (ante-hoc)

- Some models afford explanations
 - interpretable-by-design
- Examples, (generalized) linear models, decision trees, k-NN
- Example: Linear regression

$$\hat{y} = w_1 x_1 + \ldots + w_p x_p + b$$

Interpretable models (ante-hoc)

• Result in the bike sharing dataset (model weights)

$$\hat{y} = w_1 x_1 + \ldots + w_p x_p + b$$

	Weight	SE	t
(Intercept)	2399.4	238.3	10.1
seasonSPRING	899.3	122.3	7.4
seasonSUMMER	138.2	161.7	0.9
seasonFALL	425.6	110.8	3.8
holidayHOLIDAY	-686.1	203.3	3.4
workingdayWORKING DAY	124.9	73.3	1.7
weathersitMISTY	-379.4	87.6	4.3
weathersitRAIN/SNOW/STORM	-1901.5	223.6	8.5
temp	110.7	7.0	15.7
hum	-17.4	3.2	5.5
windspeed	-42.5	6.9	6.2
days_since_2011	4.9	0.2	28.5

Figure: C. Molnar, IML book, 2022 (Molnar, 2022)

Interpretable models (ante-hoc)

• Feature effects (visualization)

$$effect_j^{(i)} = w_j x_j^{(i)}$$

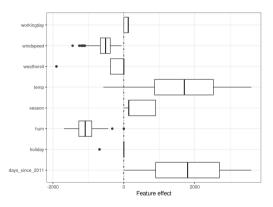


Figure: C. Molnar, IML book, 2022 Molnar, 2022

Feature effect methods (1)

- Black-box model $f(\cdot): \mathcal{X} \to \mathcal{Y}$, trained on \mathcal{D}
- Goal:
 - For single variable: Plot illustrating the effect of a feature x_s on f for all values of x_s
 - For pairs of variables: Plot illustrating the effect of pair (x_s,x_l) on f for all values of x_s and x_l

Feature Effect: global, model-agnostic, outputs plot

Feature Effect methods (2)

 $y = f(x_s) \rightarrow \text{plot}$ showing the effect of x_s on the output y

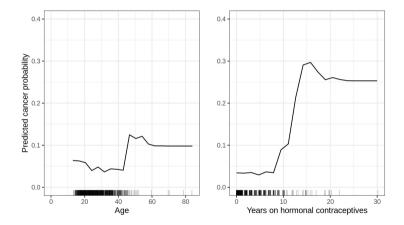


Figure: C. Molnar, IML book, 2022 (Molnar, 2022)

Feature Effect is simple and intuitive.

Feature Effect Methods (3)

- $x_s
 ightarrow$ feature of interest, $oldsymbol{x_c}
 ightarrow$ other features
- How can we isolate x_s ?
- Difficult task:
 - features are correlated
 - *f* has learned complex interactions

PDP, MPlot and ALE

- PDP (Friedman, 2001)
 - $f(x_s) = \mathbb{E}_{\boldsymbol{x_c}}[f(x_s, \boldsymbol{x_c})]$
 - Unrealistic instances

• e.g.
$$f(x_{age} = 20, x_{years_contraceptives} = 20) = ??$$

PDP, MPlot and ALE

- PDP (Friedman, 2001)
 - $f(x_s) = \mathbb{E}_{\boldsymbol{x_c}}[f(x_s, \boldsymbol{x_c})]$
 - Unrealistic instances
 - e.g. $f(x_{age} = 20, x_{years_contraceptives} = 20) = ??$
- MPlot (Apley and Zhu, 2020)
 - $\boldsymbol{x_c}|x_s: f(x_s) = \mathbb{E}_{\boldsymbol{x_c}|x_s}[f(x_s, \boldsymbol{x_c})]$
 - Aggregated effects
 - Real effect: $x_{\text{age}} = 50 \rightarrow 10$, $x_{\text{years}_contraceptives} = 20 \rightarrow 10$
 - MPlot may assign 17 to both

PDP, MPlot and ALE

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 - MPlot may assign 17 to both
- ALE (Apley and Zhu, 2020)
 - $f(x_s) = \int_{x_{min}}^{x_s} \mathbb{E}_{\boldsymbol{x_c}|z} [\frac{\partial f}{\partial x_s}(z, \boldsymbol{x_c})] \partial z$
 - Resolves both failure modes

ALE approximation

$$\begin{array}{l} \text{ALE definition: } f(x_s) = \int_{x_{s,min}}^{x_s} \mathbb{E}_{\boldsymbol{x_c}|z} [\frac{\partial f}{\partial x_s}(z, \boldsymbol{x_c})] \partial z \\ \text{ALE approximation: } f(x_s) = \sum_{k}^{k_x} \underbrace{\frac{1}{|\mathcal{S}_k|} \sum_{i: \boldsymbol{x^i} \in \mathcal{S}_k} \underbrace{[f(z_k, \boldsymbol{x_c^i}) - f(z_{k-1}, \boldsymbol{x_c^i})]}_{\text{point effect}}}_{\text{bin effect}} \end{array}$$

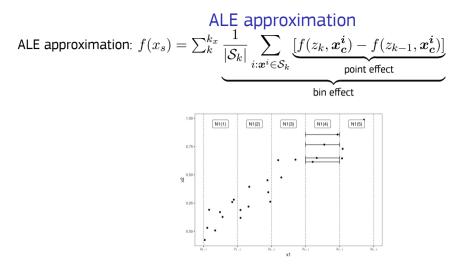


Figure: Image taken from Interpretable ML book (Molnar, 2022)

Bin splitting (parameter *K*) is crucial!

ALE approximation - weaknesses

$$f(x_s) = \sum_{k}^{k_x} \underbrace{\frac{1}{|\mathcal{S}_k|} \sum_{i: x^i \in \mathcal{S}_k} \underbrace{[f(z_k, x_c^i) - f(z_{k-1}, x_c^i)]}_{\text{point effect}}}_{\text{bin effect}}$$

- Point Effect ⇒ evaluation at bin limits
 - 2 evaluations of f per point \rightarrow slow
 - change bin limits, pay again 2*N evaluations of $f \rightarrow$ restrictive
 - broad bins may create out of distribution (OOD) samples ightarrow not-robust in wide bins

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Differential Accumulated Local Effects (DALE) Dale is faster and more versatile DALE is more Accurate

RHALE: Robust and Heterogeneity-aware Accumulated Local Effects

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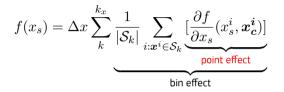
V. Gkolemis, T. Dalamagas and C. Diou, "DALE: Differential Accumulated Local Effects for efficient and accurate global explanations", ACML 2022 (Gkolemis, Dalamagas, and Diou, 2023)

Work in collaboration with Vasilis Gkolemis (PhD student @ HUA) and Theodoros Dalamagas (Researcher, ATHENA RC)





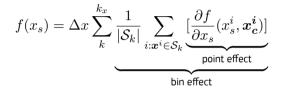
Our proposal: Differential ALE



- Point Effect \Rightarrow evaluation on instances
 - Fast \rightarrow use of auto-differentiation, all derivatives in a single pass
 - Versatile ightarrow point effects computed once, change bins without cost
 - Secure \rightarrow does not create artificial instances
 - Unbiased estimator of ALE (bias / variance proofs in the paper and supporting material)

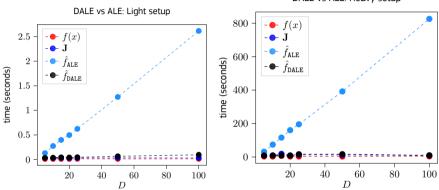
For differentiable models, DALE resolves ALE weaknesses

DALE is faster and more versatile - theory



- Faster
 - gradients wrt all features $abla_{m{x}} f(m{x^i})$ in a single pass (via the Jacobian)
 - auto-differentiation must be available (deep learning)
- Versatile
 - Change bin limits, with near zero computational cost
- DALE is faster and allows redefintion of the bin limits

DALE is faster and versatile - Experiments

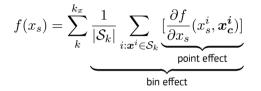


DALE vs ALE: Heavy setup

Figure: Light setup; small dataset ($N = 10^2$ instances), computationally light f. Heavy setup; big dataset ($N = 10^5$ instances), computationally heavy f. D is the number of dimensions.

DALE considerably accelerates the estimation

DALE uses on-distribution samples - Theory



- point effect independent of bin limits
 - $\frac{\partial f}{\partial x_s}(x^i_s, x^i_c)$ computed on real instances $x^i = (x^i_s, x^i_c)$
- bin limits affect only the resolution of the plot
 - wide bins ightarrow low resolution plot, bin estimation from more points
 - narrow bins ightarrow high resolution plot, bin estimation from less points

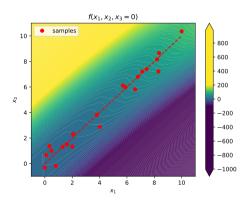
DALE enables wide bins without creating out of distribution instances

DALE uses on-distribution samples - Experiments

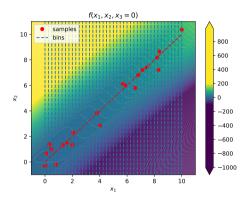
$$f(x_1, x_2, x_3) = x_1 x_2 + x_1 x_3 \pm g(x)$$
$$x_1 \in [0, 10], x_2 \sim x_1 + \epsilon, x_3 \sim \mathcal{N}(0, \sigma^2)$$
$$f_{ALE}(x_1) = \frac{x_1^2}{2}$$

- point effects affected by (x_1x_3) (σ is large)
- bin estimation is noisy (samples are few)

Intuition: we need wider bins (more samples per bin)

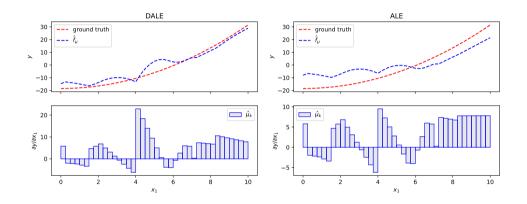


DALE vs ALE - 40 Bins



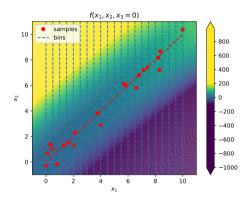
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
- ALE: on-distribution, noisy bin effect \rightarrow poor estimation

DALE vs ALE - 40 Bins



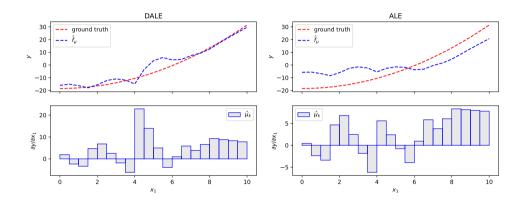
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
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DALE vs ALE - 20 Bins



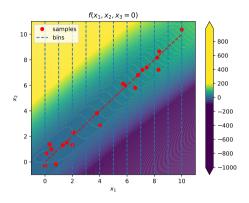
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
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DALE vs ALE - 20 Bins



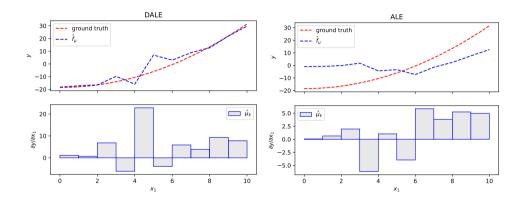
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
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DALE vs ALE - 10 Bins



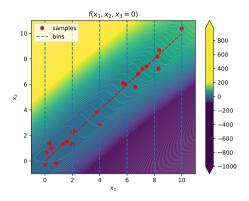
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
- ALE: starts being OOD, noisy bin effect \rightarrow poor estimation

DALE vs ALE - 10 Bins



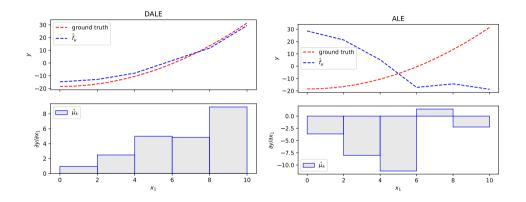
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
- ALE: starts being OOD, noisy bin effect \rightarrow poor estimation

DALE vs ALE - 5 Bins



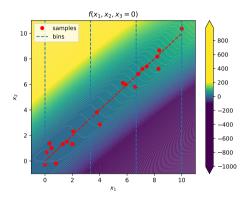
- DALE: on-distribution, robust bin effect \rightarrow good estimation
- ALE: completely OOD, robust bin effect \rightarrow poor estimation

DALE vs ALE - 5 Bins



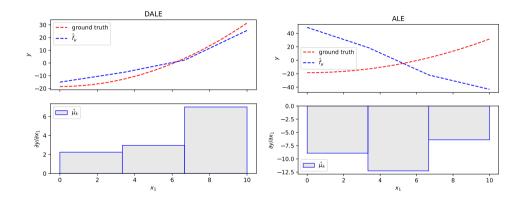
- DALE: on-distribution, robust bin effect \rightarrow good estimation
- ALE: completely OOD, robust bin effect \rightarrow poor estimation

DALE vs ALE - 3 Bins



- DALE: on-distribution, robust bin effect \rightarrow good estimation
- ALE: completely OOD, robust bin effect \rightarrow poor estimation

DALE vs ALE - 3 Bins



- DALE: on-distribution, robust bin effect \rightarrow good estimation
- ALE: completely OOD, robust bin effect \rightarrow poor estimation

Real Dataset Experiments - Efficiency

- Bike-sharing dataset (Fanaee-T and Gama, 2013)
- $y \rightarrow \text{daily bike rentals}$
- x: 10 features, most of them characteristics of the weather

	Number of Features										
	1	2	3	4	5	6	7	8	9	10	11
DALE	1.17	1.19	1.22	1.24	1.27	1.30	1.36	1.32	1.33	1.37	1.39
ALE	0.85	1.78	2.69	3.66	4.64	5.64	6.85	7.73	8.86	9.9	10.9

Efficiency on Bike-Sharing Dataset (Execution Times in seconds)

DALE requires almost same time for all features

Real Dataset Experiments - Accuracy

- Difficult to compare in real world datasets
- We do not know the ground-truth effect
- In most features, DALE and ALE agree.
- Only X_{hour} is an interesting feature

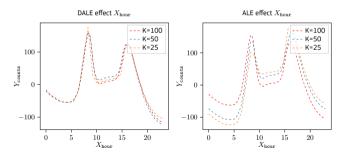


Figure: (Left) DALE (Left) and ALE (Right) plots for $K = \{25, 50, 100\}$

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V. Gkolemis, T. Dalamagas, E. Ntoutsi and C. Diou, "RHALE: Robust and Heterogeneity-aware Accumulated Local Effects ", ECAI 2023 (Gkolemis, Dalamagas, Ntoutsi, et al., 2023)

Work in collaboration with Vasilis Gkolemis (PhD student @ HUA), Theodoros Dalamagas (Researcher, ATHENA RC) and Eirini Ntoutsi (Prof, Universität der Bundeswehr, München)



Next step: Heterogeneity and optimal bin selection

Using DALE, one has the computational margin to worry about additional issues:

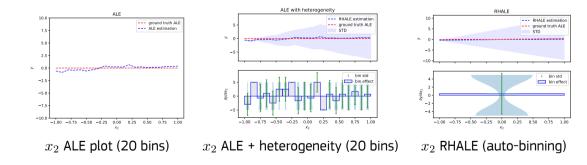
- Computation of heterogeneity of local effects (i.e., standard error of the mean)
- Optimal selection of bins such that the effect does not have a high variation within the bin
- RHALE: Robust and Heterogeneity-aware Accumulated Local Effects
 - Robust: Automatic bin splitting (result does not depend on arbitrary bin selection)
 - Heterogeneity aware: \pm from the average

Example (based on Goldstein et al., 2015)

Aggregation bias

$$Y = 0.2X_1 - 5X_2 + 10X_2 \mathbb{1}_{X_3 > 0} + \mathcal{E}$$

$$\mathcal{E} \stackrel{i.i.d.}{\sim} \mathcal{N}(0,1), \quad X_1, X_2, X_3 \stackrel{i.i.d.}{\sim} \mathcal{U}(-1,1)$$



Definitions and Approximations - Main effect

ALE main effect definition

$$f^{\text{ALE}}(x_s) = \int_{x_{s,\min}}^{x_s} \underbrace{\mathbb{E}_{X_c \mid X_s = z} \left[f^s(z, X_c) \right]}_{\mu(z)} \partial z$$

ALE main effect approximation

$$\hat{f}^{\text{ALE}}(x_s) = \Delta x \sum_{k}^{k_x} \underbrace{\frac{1}{|\mathcal{S}_k|} \sum_{i: \boldsymbol{x}^i \in \mathcal{S}_k} [\frac{\partial f}{\partial x_s}(x_s^i, \boldsymbol{x}_c^i)]}_{\text{bin effect}: \hat{\boldsymbol{\mu}}(z)}$$

Simple but wrong: ALE + Heterogeneity

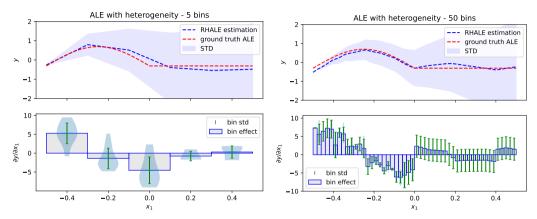


Figure: Left: approximation with narrow bin-splitting (5 bins) and (Right) with dense-bin splitting

• Fixed-size bin splitting can ruin the estimation of the heterogeneity

Definitions and Approximations - Heterogeneity

ALE heterogeneity definition

$$\sigma(x_s) = \sqrt{\int_{x_{s,\min}}^{x_s} \underbrace{\mathbb{E}_{X_c|X_s=z}\left[\left(f^s(z,X_c) - \mu(z)\right)^2\right] \partial z}_{\sigma^2(z)}}$$

ALE heterogeneity approximation

$$STD(x_s) = \sqrt{\sum_{k=1}^{k_x} (z_k - z_{k-1})^2 \underbrace{\frac{1}{|\mathcal{S}_k| - 1} \sum_{i: \mathbf{x}^i \in \mathcal{S}_k} \left(f^s(\mathbf{x}^i) - \hat{\mu}(z_{k-1}, z_k) \right)^2}_{\sigma^2(z)}}_{\sigma^2(z)}$$

Derivations

In the paper we formally prove

- 1. the conditions under which the above definition is an unbiase estimator of the heterogeneity
- 2. the conditions under which a bin splitting minimizes the estimator variance

Based on the above, we formulate bin-splitting as an optimization problem and propose an efficient solution using dynamic programming.

RHALE: Robust and Heterogeneity-aware ALE

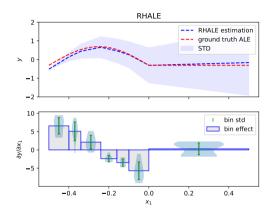


Figure: Variable bin size leads to improved estimation

Simple but correct:

- Automatically finds the **optimal** bin-splitting
- Optimal ⇒ best approximation of the average (ALE) effect
- Optimal ⇒ best approximation of the heterogeneity

Impact

In case you work with a differentiable model, as in Deep Learning, use the combination of DALE and RHALE to:

- compute ALE fast, for multiple bin sizes in one pass
- quantify the heterogeneity of the ALE plot, i.e., the deviation of the instance-level effects from the average effect
- get a robust approximation of (a) the main ALE effect and (b) the heterogeneity, using automatic bin-splitting

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Effector - A python package for global and regional feature effects

V. Gkolemis, C. Diou, V. Gkolemis, C. Diou, E. Ntoutsi, T. Dalamagas, B. Bischl, J. Herbinger, G. Casalicchio, "Effector: A Python package for regional explanations", arXiv preprint arXiv:2404.02629, 2024

https://xai-effector.github.io

Installation, for python version 3.7+:

pip install effector

Regional effects

• Similar to the way one can select optimal bin splits to minimize heterogeneity, one can also identify optimal subregions of the features x_c where the effect is homogeneous

Regional effect plots - Process

- Combines two methods:
 - RHALE
 - Regional effects (Herbinger, Bischl, and Casalicchio, 2023)
- Idea:
 - Feature effect is the average effect of each feature x_s on the output y
 - It is computed by averaging the instance-level effects
 - Heterogeneity ${\cal H}$ measures the deviation of the instance-level effects from the average effect due to feature interactions
 - Split the dataset in subgroups in order to minimize the heterogeneity
- Concretely:

$$\underbrace{\mathcal{H}(f_i(x_i))}_{\mathcal{H}(f_i(x_i|x_j > \tau)) + \mathcal{H}(f_i(x_i|x_j \le \tau))} \underbrace{\mathcal{H}(f_i(x_i|x_j \le \tau))}_{\mathcal{H}(f_i(x_i|x_j \le \tau)) + \mathcal{H}(f_i(x_i|x_j \le \tau))}$$

 ${\mathcal H}$ before split

sum of ${\mathcal H}$ after split

Regional effect plots - Objective

$$\begin{array}{ll} \underset{\{\mathcal{R}_{st}\}_{t=1}^{T_s}}{\text{minimize}} & \mathcal{L}_s = \sum_{t=1}^{T_s} \frac{|\mathcal{D}_{st}|}{|\mathcal{D}|} H_{st}^{\mathtt{m}} \\ \text{subject to} & \bigcup_{t=1}^{T} \mathcal{R}_{st} = \mathcal{X}_c \\ & \mathcal{R}_{st} \cap \mathcal{R}_{s\tau} = \emptyset, \quad \forall t \neq \tau \end{array}$$

(1)

Algorithm

Algorithm 1: Detect subspaces

```
Input : Heterogeneity function H_{s}. Maximum depth L
   Output: subspaces \{\mathcal{R}_{st}\}_{t=1}^{T_s}, where T_s \in \{0, 2, \dots, 2^L\}
1 H<sub>s0</sub>;
                                                                                  // Compute the level of interactions before any split
2 D = \{(\mathbf{x}^i, y^i)\}_{i=1}^N;
                                                                                                                                    // Initial dataset
3 T_s = 0;
                                                                                         // Initialize the number of splits for feature s
4 for l = 1 to L do
          if H_{a}^{l-1} = 0 then
                break :
                                                                                                          // Stop if the heterogeneity is zero
 6
7
          end
          /* Iterate over all features \mathbf{x}_c and candidate split positions p
                                                                                                                                                           * /
          /* Find the optimal split with heterogeneity H_s^l = \sum_{t=1}^{2^l} \frac{|\mathcal{D}_{st}|}{|\mathcal{D}|} H_{st}
                                                                                                                                                           */
          /* Define the subspaces \{\mathcal{R}_{st}\}_{t=1}^{2^l} and the datasets \{\mathcal{D}_{st}\}_{t=1}^{2^l}
                                                                                                                                                           */
         if rac{H_s^l}{rl-1} < \epsilon then
8
              break ;
                                                                                             // Stop. if heterogeneity drop is small (< \epsilon)
9
          and
10
          T_{a} = 2^{l}
                                                                                               // Update the number of splits for feature s
11
12
    end
   return {\mathcal{R}_{st} | s \in \{1, \ldots, D\}, t \in \{1, \ldots, T_s\}}
13
```

Effector - Implemented methods

Method	Equation	Formula				
$\hat{f}^{\text{RHALE}}(x_s)$	Eq. (4)	$\sum_{k=1}^{kx_{x_s}} \frac{z_k - z_{k-1}}{ \mathcal{S}_k } \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} \frac{\partial f}{\partial x_s}(x_s^i, \mathbf{x}_c^i)$				
$\hat{H}^{\mathrm{RHALE}}_s$	Eq. (6)	$\sum_{k=1}^{K_s} \frac{z_k - z_{k-1}}{ \mathcal{S}_k } \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} \left[\frac{\partial f}{\partial x_s} (x_s^i, \mathbf{x}_c^i) - \hat{\mu}_k^{\text{RHALE}} \right]^2$				
$\hat{f}^{\rm ALE}(x_s)$	Eq. (3)	$\sum_{k=1}^{k_{x_s}} \frac{1}{ \mathcal{S}_k } \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} \left[f(z_k, \mathbf{x}_c^i) - f(z_{k-1}, \mathbf{x}_c^i) \right]$				
$\hat{H}^{\rm ALE}_s$	Eq. (5)	$\sum_{k=1}^{K} \frac{1}{ \mathcal{S}_k } \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} \left[(f(z_k, \mathbf{x}_c^i) - f(z_{k-1}, \mathbf{x}_c^i)) - \hat{\mu}_k^{ALE} \right]^2$				
$\hat{f}^{\rm PDP}(x_s)$	Eq. (7)	$\frac{1}{N}\sum_{i=1}^{N}f(x_s, \mathbf{x}_c^i)$				
$\hat{H}^{\rm PDP}_s$	Eq. (8)	$\frac{1}{T}\sum_{t=1}^T \frac{1}{N}\sum_{i=1}^N \left[\hat{f}_{i,\text{centered}}^{\text{ICE}}(x_{s,t}) - \hat{f}_{\text{centered}}^{\text{PDP}}(x_{s,t}) \right]^2$				
$\hat{f}^{\mathbf{d}-\mathbf{PDP}}(x_s)$	Eq. (9)	$\frac{1}{N}\sum_{i=1}^{N}f(x_s,\mathbf{x}_c^i)$				
$\hat{H}^{\rm d-PDP}_s$	Eq. (10)	$\frac{1}{T} \sum_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \left[\hat{f}_{i,\text{centered}}^{\text{ICE}}(x_{s,t}) - \hat{f}_{\text{centered}}^{\text{PDP}}(x_{s,t}) \right]^2$				
$\hat{f}^{\texttt{SHAP}-\texttt{DP}}(x_s)$	Eq. (13)	$\kappa(x_s), \kappa(x_s)$ is a univariate spline fit to $\{(x_s^i, \hat{\phi}_s^i)\}_{i=1}^N$				
$\hat{H}_s^{\texttt{SHAP-DP}}$	Eq. (14)	$\frac{1}{N}\sum_{i=1}^{N}\left[\hat{\phi}_{s}^{i}-f^{\texttt{SHAP}-\texttt{DP}}(x_{s}^{i})\right]^{2}$				

Effector - Tutorial

Tutorial (Bike Sharing Dataset) Colab notebook

Recap

- DALE can help with the computation of fast and accurate feature effect explanations for differentiable models
 - One can change the resolution of the explanation (i.e., number of bins K) for free
- RHALE can improve explanations by selecting variable bin splits, in an optimal way
 - Unbiased estimation of heterogeneity
 - Select optimal bin splits to minimize heterogeneity and improve the robustness of the explanation
- Effector
 - Implements all popular global effect plot methods
 - Extends these methods to regional effect plots
 - Has very fast implementation, especially for differentiable models (takes advantage of auto-differentiation)

Thank you!

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