



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

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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/

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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

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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

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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

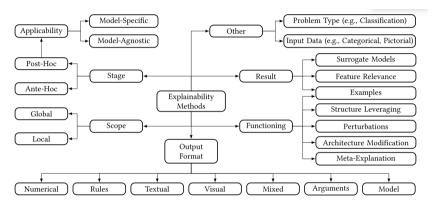


Figure: Timo Speith, "A Review of Taxonomies of Explainable Artificial Intelligence (XAI) Methods". In 2022 ACM Conference on Fairness, Accountability, and Transparency (FAccT '22), 2022 (Speith, 2022)

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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)

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

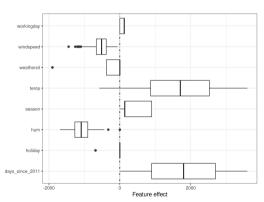


Figure: C. Molnar, IML book, 2022 Molnar, 2022

Feature effect methods (1)

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

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

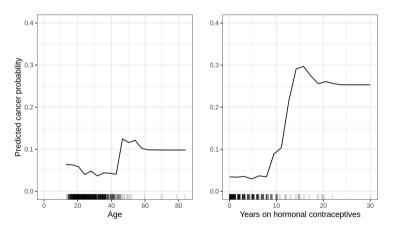


Figure: C. Molnar, IML book, 2022 (Molnar, 2022)

Feature Effect is simple and intuitive.

Feature Effect Methods (3)

- $x_s o$ feature of interest, $x_c o$ 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. $f(x_{\text{age}} = 20, x_{\text{years_contraceptives}} = 20) = ??$

PDP, MPlot and ALE

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 - Unrealistic instances
 - e.g. $f(x_{\text{age}} = 20, x_{\text{years_contraceptives}} = 20) = ??$
- 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: $x_{\text{age}} = 50 \rightarrow 10$, $x_{\text{vears contraceptives}} = 20 \rightarrow 10$
 - MPlot may assign 17 to both

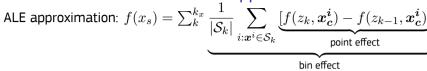
PDP, MPlot and ALE

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

ALE approximation

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

ALE approximation



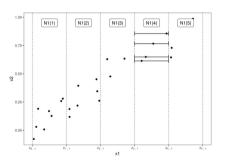


Figure: Image taken from Interpretable ML book (Molnar, 2022)

Bin splitting (parameter K) is crucial!

ALE approximation - weaknesses

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

- Point Effect ⇒ evaluation at bin limits
 - 2 evaluations of f per point \rightarrow slow
 - change bin limits, pay again 2*N evaluations of $f \to \text{restrictive}$
 - ullet broad bins may create out of distribution (OOD) samples o 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 Effect

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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

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

- Point Effect ⇒ evaluation on instances
 - Fast \rightarrow use of auto-differentiation, all derivatives in a single pass
 - Versatile → point effects computed once, change bins without cost
 - Secure → 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

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

- Faster
 - gradients wrt all features $\nabla_{x} f(x^{i})$ 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

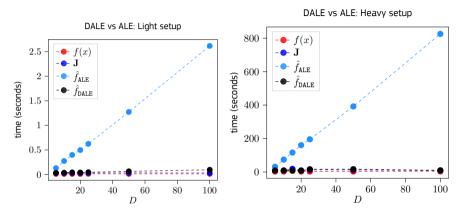


Figure: Light setup; small dataset ($N=10^2$ instances), computationally light f. Heavy setup; big dataset ($N=10^5$ instances), computationally heavy f. D is the number of dimensions.

DALE considerably accelerates the estimation

DALE uses on-distribution samples - Theory

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

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

DALE enables wide bins without creating out of distribution instances

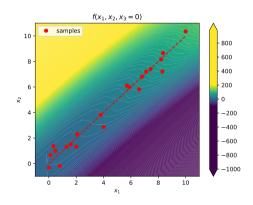
DALE uses on-distribution samples - Experiments

$$f(x_1, x_2, x_3) = x_1 x_2 + x_1 x_3 \pm g(x)$$

$$x_1 \in [0, 10], x_2 \sim x_1 + \epsilon, x_3 \sim \mathcal{N}(0, \sigma^2)$$

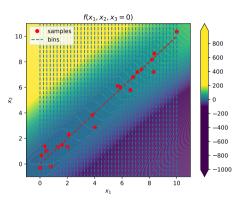
$$f_{\text{ALE}}(x_1) = \frac{x_1^2}{2}$$

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



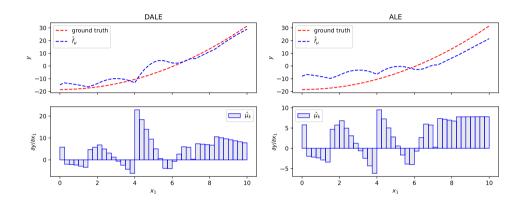
Intuition: we need wider bins (more samples per bin)

DALE vs ALE - 40 Bins



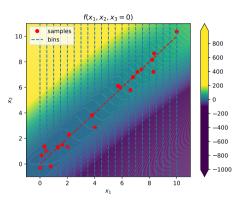
- DALE: on-distribution, noisy bin effect → poor estimation
- ullet ALE: on-distribution, noisy bin effect ightarrow poor estimation

DALE vs ALE - 40 Bins



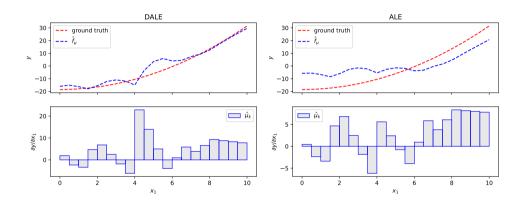
- DALE: on-distribution, noisy bin effect → poor estimation
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DALE vs ALE - 20 Bins



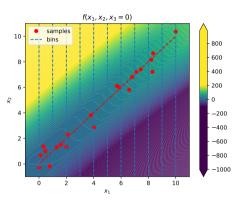
- DALE: on-distribution, noisy bin effect → poor estimation
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DALE vs ALE - 20 Bins



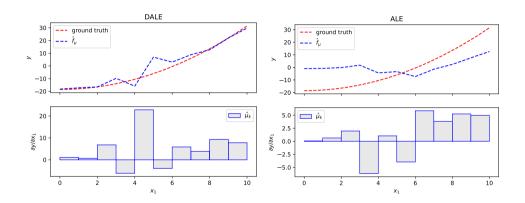
- DALE: on-distribution, noisy bin effect \rightarrow poor estimation
- ullet ALE: on-distribution, noisy bin effect ightarrow poor estimation

DALE vs ALE - 10 Bins



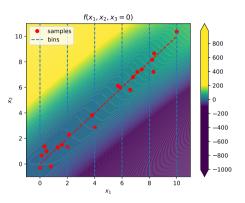
- DALE: on-distribution, noisy bin effect → poor estimation
- ALE: starts being OOD, noisy bin effect \rightarrow poor estimation

DALE vs ALE - 10 Bins



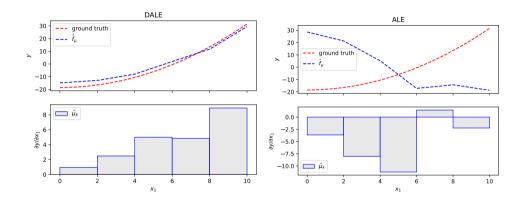
- DALE: on-distribution, noisy bin effect → poor estimation
- ALE: starts being OOD, noisy bin effect \rightarrow poor estimation

DALE vs ALE - 5 Bins



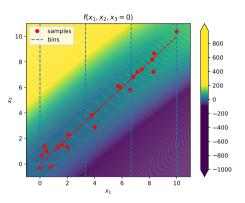
- DALE: on-distribution, robust bin effect → good estimation
- ALE: completely OOD, robust bin effect \rightarrow poor estimation

DALE vs ALE - 5 Bins



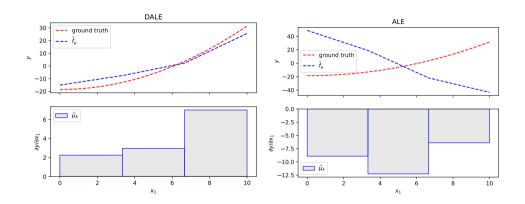
- DALE: on-distribution, robust bin effect → good estimation
- ullet ALE: completely OOD, robust bin effect ightarrow poor estimation

DALE vs ALE - 3 Bins



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

DALE vs ALE - 3 Bins



- DALE: on-distribution, robust bin effect → good estimation
- ullet ALE: completely OOD, robust bin effect ightarrow poor estimation

Real Dataset Experiments - Efficiency

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

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

	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

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

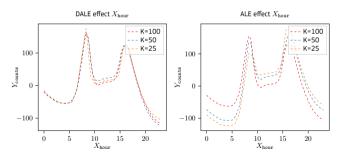


Figure: (Left) DALE (Left) and ALE (Right) plots for $K=\{25,50,100\}$

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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

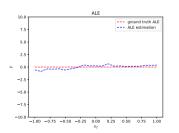
- Robust: Automatic bin splitting (result does not depend on arbitrary bin selection)
- ullet Heterogeneity aware: \pm from the average

Example (based on Goldstein et al., 2015)

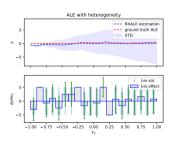
Aggregation bias

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

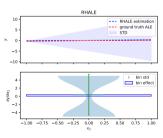
$$\mathcal{E} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1), \quad X_1, X_2, X_3 \stackrel{i.i.d.}{\sim} \mathcal{U}(-1, 1)$$



 x_2 ALE plot (20 bins)



 x_2 ALE + heterogeneity (20 bins)



 x_2 RHALE (auto-binning)

Definitions and Approximations - Main effect

ALE main effect definition

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

ALE main effect approximation

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

Simple but wrong: ALE + Heterogeneity

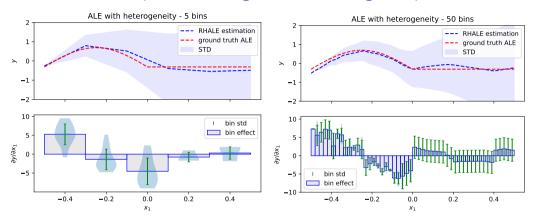


Figure: Left: approximation with narrow bin-splitting (5 bins) and (Right) with dense-bin splitting

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

Definitions and Approximations - Heterogeneity

ALE heterogeneity definition

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

ALE heterogeneity approximation

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

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

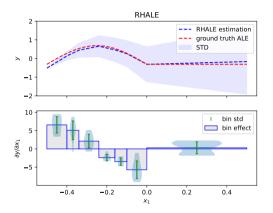


Figure: Variable bin size leads to improved estimation

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

ullet Similar to the way one can select optimal bin splits to minimize heterogeneity, one can also identify optimal subregions of the features $m{x}_c$ 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:

$$\underbrace{\mathcal{H}(f_i(x_i))}_{\mathcal{H} \text{ before split}} >> \underbrace{\mathcal{H}(f_i(x_i|x_j > \tau)) + \mathcal{H}(f_i(x_i|x_j \leq \tau))}_{\text{sum of } \mathcal{H} \text{ after split}}$$

Regional effect plots - Objective

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
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
7
         /st Iterate over all features \mathbf{x_c} and candidate split positions p
                                                                                                                                                        * /
         /* Find the optimal split with heterogeneity H_s^l = \sum_{t=1}^{2l} \frac{|\mathcal{D}_{st}|}{|\mathcal{D}|} H_{st}
                                                                                                                                                        */
         /* Define the subspaces \{\mathcal{R}_{st}\}_{t=1}^{2l} and the datasets \{\mathcal{D}_{st}\}_{t=1}^{2l}
                                                                                                                                                        * /
        if rac{H_s^l}{l^{l-1}}<\epsilon then
             ° break ;
                                                                                            // Stop. if heterogeneity drop is small (< \epsilon)
         T_a = 2^l
                                                                                             // Update the number of splits for feature s
   return \{\mathcal{R}_{st} | s \in \{1, \dots, D\}, t \in \{1, \dots, T_s\}\}
```

Effector - Implemented methods

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

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)



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