Paper presentation at ACML 2022

DALE: Differential Accumulated Local Effects for efficient and accurate global explanations

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eXplainable AI (XAI)

- Black-box model $f(\cdot) : \mathcal{X} \rightarrow \mathcal{Y}$, trained on $\mathcal{D}$
- XAI extracts interpretable properties:
  - $\rightarrow$ Which features are important (in general)?
  - $\rightarrow$ Which features favor a prediction?
- Categories:
  - $\rightarrow$ Global vs local
  - $\rightarrow$ Model-agnostic vs Model-specific
  - $\rightarrow$ Output? number, plot, instance etc.

Feature Effect: global, model-agnostic, outputs plot

Feature Effect

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

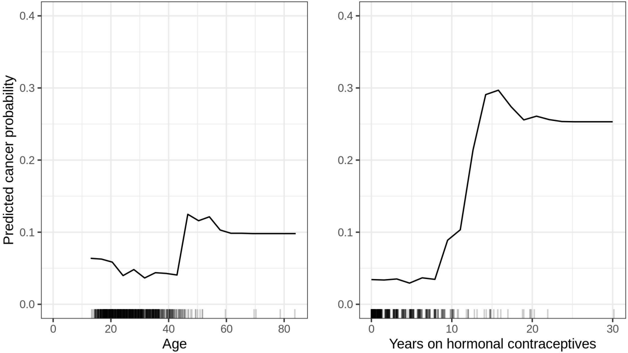

Figure: Image taken from Interpretable ML book [4]

Feature Effect is simple and intuitive.

Feature Effect Methods

- $x_s \rightarrow$ feature of interest, $\boldsymbol{x_c} \rightarrow$ other features
- FE methods take $(f, \mathcal{D}, s)$ and return $y = f_{<\texttt{name}>}(x_s)$
- PDP[3]
    - Expected outcome over $\boldsymbol{x_c}$: $f(x_s) = \mathbb{E}_{\boldsymbol{x_c}}[f(x_s, \boldsymbol{x_c})]$
    - **Unrealistic instances**

PDP vs MPlot vs ALE

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  - **Unrealistic instances**
- MPlot[1]
  - Expected outcome over $\boldsymbol{x_c}|x_s$: $f(x_s) = \mathbb{E}_{\boldsymbol{x_c}|x_s}[f(x_s, \boldsymbol{x_c})]$
  - **Aggregated effects**

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  - **Aggregated effects**
- ALE[1]
  - $f(x_s) = \int_{x_{min}}^{x_s} \mathbb{E}_{\boldsymbol{x_c}|z}[\frac{\partial f}{\partial x_s}(z, \boldsymbol{x_c})]\partial z$
  - **Resolves both failure modes**

PDP vs MPlot vs ALE

ALE approximation

ALE definition: $f(x_s) = \int_{x_{s,min}}^{x_s} \mathbb{E}_{\mathbf{x_c}|z}[\frac{\partial f}{\partial x_s}(z, \mathbf{x_c})]\partial z$

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

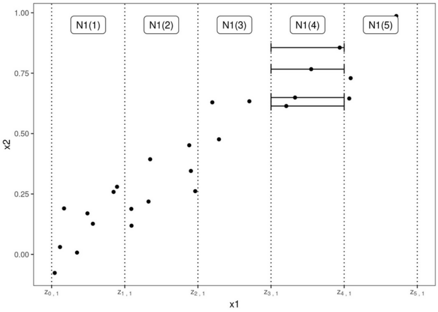

Figure: Image taken from Interpretable ML book [4]

ALE approximation

ALE approximation from $\mathcal{D} = \{\boldsymbol{x}^i, y^i\}_{i=1}^N$

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

- 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 $\rightarrow$ not-robust in wide bins

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ALE approximation has some weaknesses

DALE - Differential ALE

DALE, from the dataset $\mathcal{D} = \{\boldsymbol{x}^i, y^i\}_{i=1}^N$

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

- only change point effect computation
- Fast $\rightarrow$ use of auto-differentiation, all derivatives in a single pass
- Versatile $\rightarrow$ point effects computed once, change bins without cost
- Secure $\rightarrow$ does not create artificial instances

For differentiable models, DALE resolves ALE weaknesses

DALE is faster and versatile - theory

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

- Faster
  - gradients wrt all features $\nabla_{\boldsymbol{x}} f(\boldsymbol{x^i})$ in a single pass
  - auto-differentiation must be available (deep learning)
- Versatile
  - Change bin limits, with near zero computational cost

DALE is faster and allows redefining bin-limits

DALE is faster and versatile - Experiments

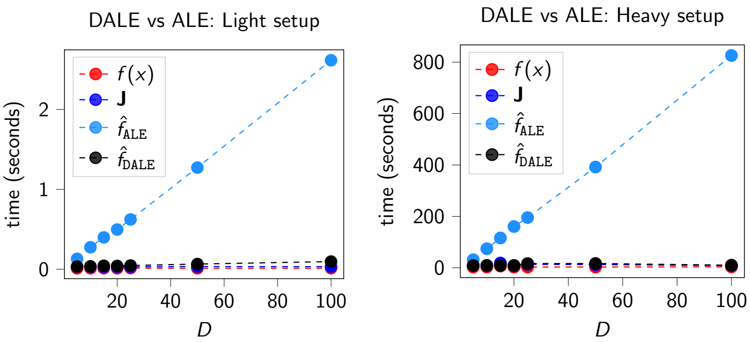


Figure: Light setup; small dataset ($N = 10^2$ instances), light f. Heavy setup; big dataset ($N = 10^5$ instances), heavy f

DALE considerably accelerates the estimation

DALE uses on-distribution samples - Theory

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

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

DALE enables wide bins without creating out of distribution instances

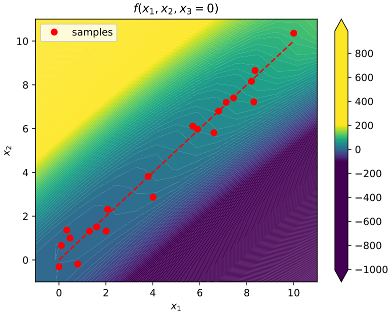
DALE uses on-distribution samples - Experiments

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

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

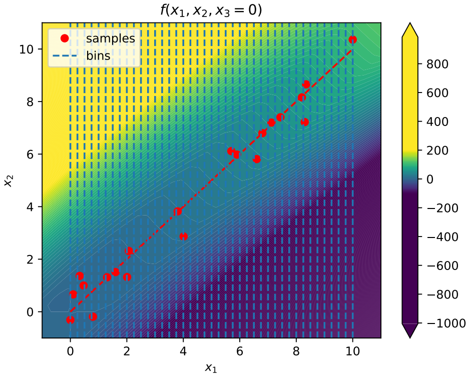
$$f_{\texttt{ALE}}(x_1) = \frac{x_1^2}{2}$$

- point effects affected by $(x_1 x_3)$ (σ is large)
- bin estimation is noisy (samples are few)



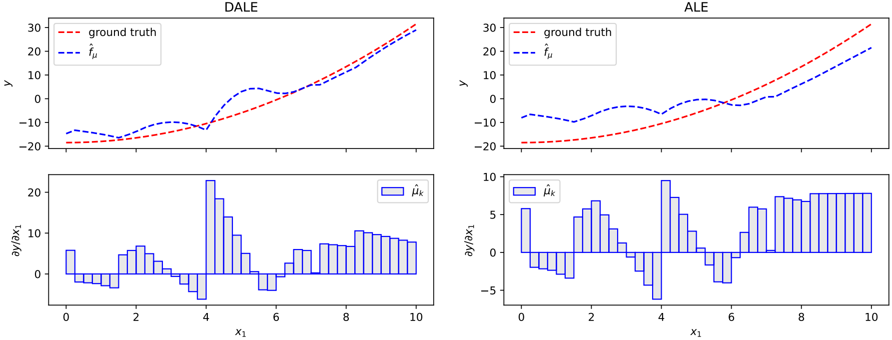
Intuition: we need wider bins (more samples per bin)

DALE vs ALE - 40 Bins



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

DALE vs ALE - 40 Bins



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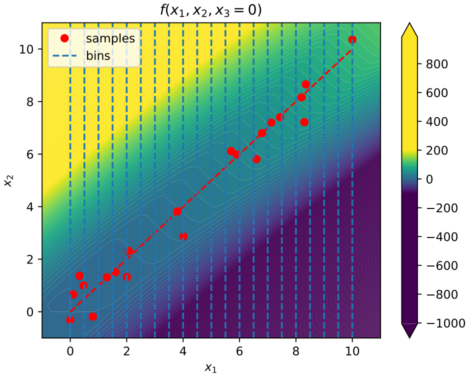
DALE vs ALE - 20 Bins



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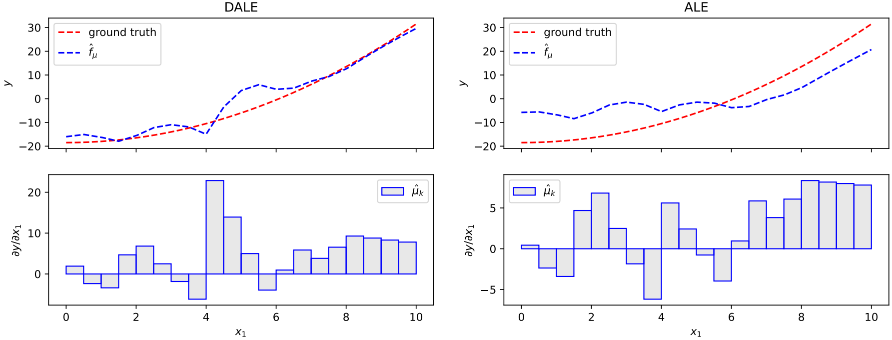
DALE vs ALE - 20 Bins



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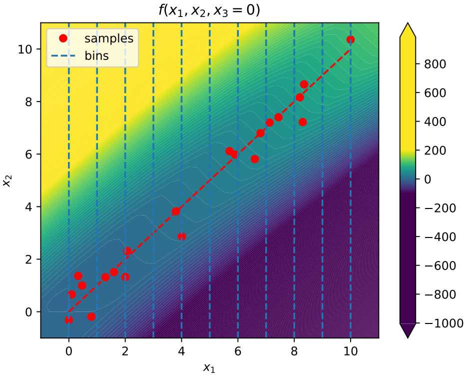
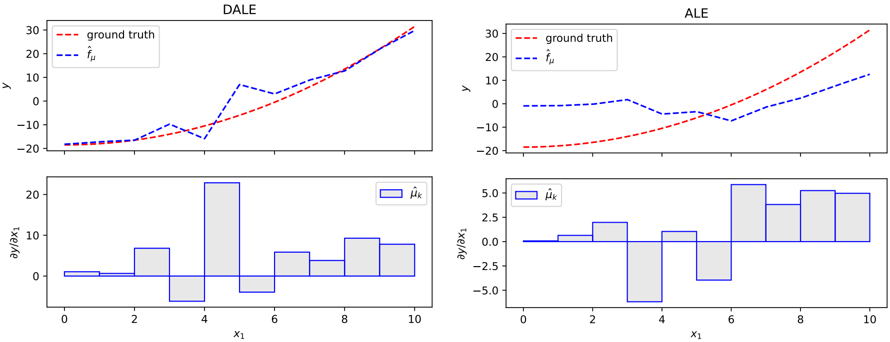
DALE vs ALE - 10 Bins



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

DALE vs ALE - 10 Bins



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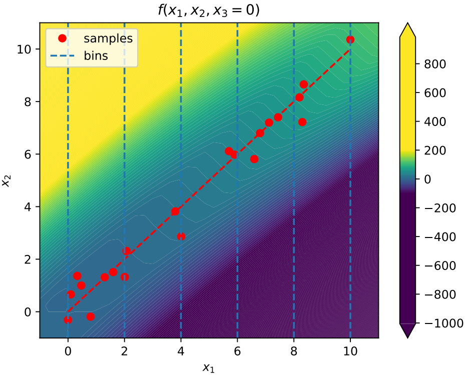
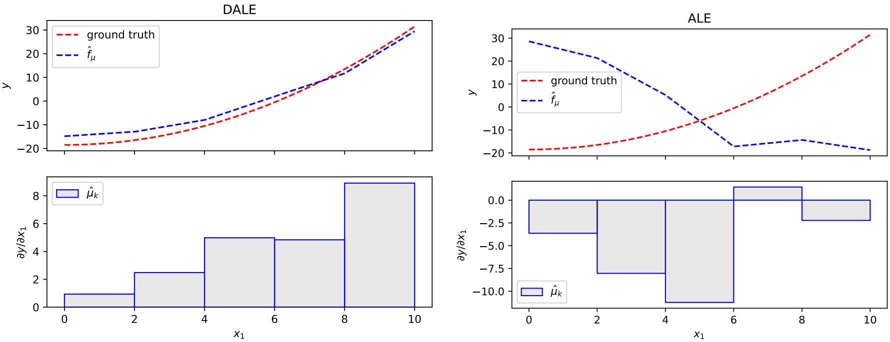
DALE vs ALE - 5 Bins



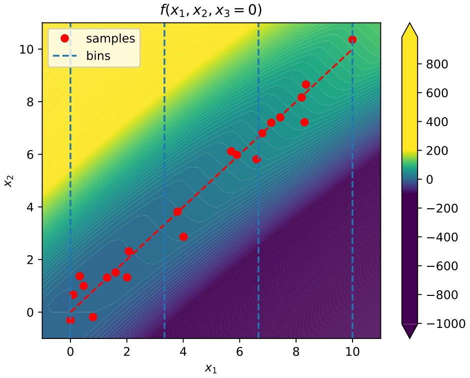
- DALE: on-distribution, robust bin effect → good estimation
- ALE: completely OOD, robust bin effect → poor estimation

DALE vs ALE - 5 Bins



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

DALE vs ALE - 3 Bins



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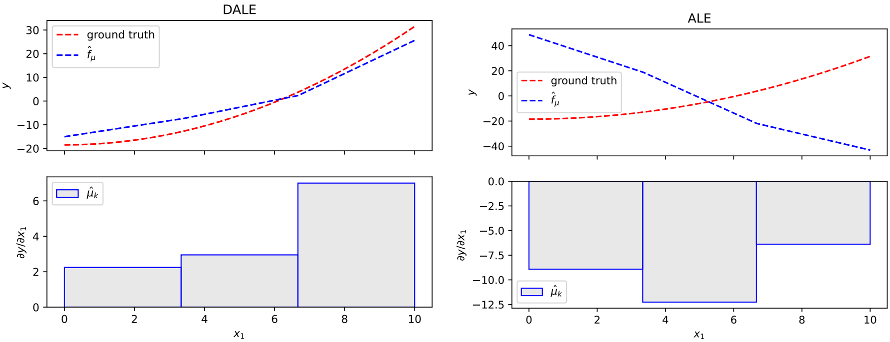
DALE vs ALE - 3 Bins



- DALE: on-distribution, robust bin effect → good estimation
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Real Dataset Experiments - Efficiency

- Bike-sharing dataset[2]
- $y \rightarrow$ daily bike rentals
- $\boldsymbol{x}$: 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 $X_{\texttt{hour}}$ is an interesting feature

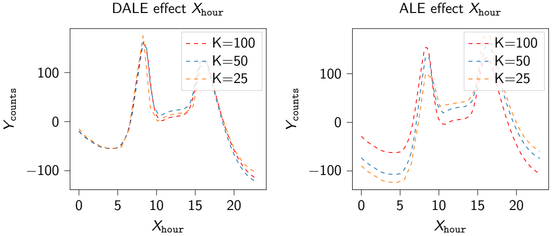

Figure: (Left) DALE (Left) and ALE (Right) plots for $K = \{25, 50, 100\}$

What next?

- How to (automatically) decide the optimal bin sizes?
  - Sometimes narrow bins are ok
  - Sometimes wide bins are needed
- Can we DALE are fast to decide optimal bin splitting?
- What about variable size bins?
- Model the uncertainty of the estimation?

DALE advantages can be a driver for future work

Thank you

- Questions?

References I

[1] Daniel W. Apley and Jingyu Zhu. Visualizing the effects of predictor variables in black box supervised learning models. *Journal of the Royal Statistical Society. Series B: Statistical Methodology*, 82(4):1059–1086, 2020.

[2] Hadi Fanaee-T and Joao Gama. Event labeling combining ensemble detectors and background knowledge. *Progress in Artificial Intelligence*, pages 1–15, 2013.

[3] Jerome H. Friedman. Greedy function approximation: A gradient boosting machine. *Annals of Statistics*, 29(5):1189–1232, oct 2001.

[4] Christoph Molnar. *Interpretable Machine Learning*. 2 edition, 2022.