DALE: Differential Accumulated Local Effects for accurate and efficient global effect estimation

Vasilis Gkolemis [1, 2] Theodore Dalamagas [1] Christos Diou [2]

[1]ATHENA Research Center [2]Harokopio University of Athens

TL;DR

DALE is a better approximation to ALE, the SotA feature effect method. By better, we mean faster and more accurate.

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Motivation

Feature effect methods are simple and intuitive; they isolate the impact of a single feature x_s in the output y. Inspecting the feature effect plot a non-expert can easily understand whether a feature has positive/negative on the target variable. The task is difficult; isolating the effect of a single variable is tricky when features are correlated and the black-box function has learned complex. ALE Apley and Zhu 2020 is the only method that manages. However, ALE estimation, i.e., the approximation of ALE from the set of has efficiency and accuracy that we address with DALE.

DALE vs ALE

ALE definition

$$f(x_s) = \int_{x_{s,min}}^{x_s} \mathbb{E}_{\boldsymbol{x_c}|z} \underbrace{[\frac{\partial f}{\partial x_s}(z, \boldsymbol{x_c})]}_{\text{point effect}} \partial z$$

ALE defines the effect at $x_s = z$ as the expected change (derivative) on the output over the conditional distribution $\boldsymbol{x_c}|z$ and the feature effect plot as the integration of the expected changes.

ALE approximation

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

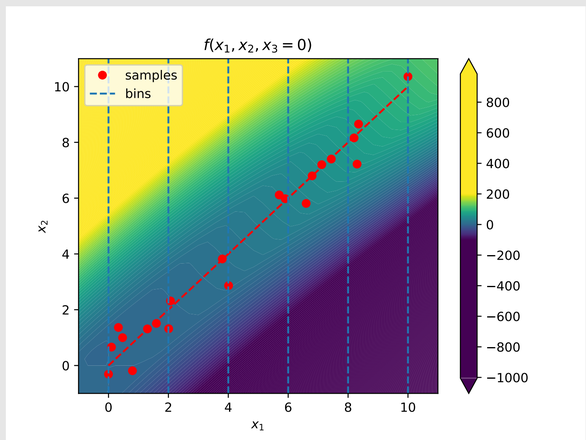
ALE approximation, i.e. estimating ALE from the training set $\mathcal{D}$, requires partitioning the s-th axis, i.e. $[x_{s,min}, x_{s,max}]$, in K equisized bins and computes the *local* point effects by evaluating the bin limits $[f(z_k, \boldsymbol{x_c^i}) - f(z_{k-1}, \boldsymbol{x_c^i})]$. This approach is slow and vulnerable to misestimatons. First, it is slow as the dimensionality of the dataset grows larger. Second, it demands predifing the bin limits. Finally, it may create out-of-distribution samples when bin size becomes large.

DALE approximation

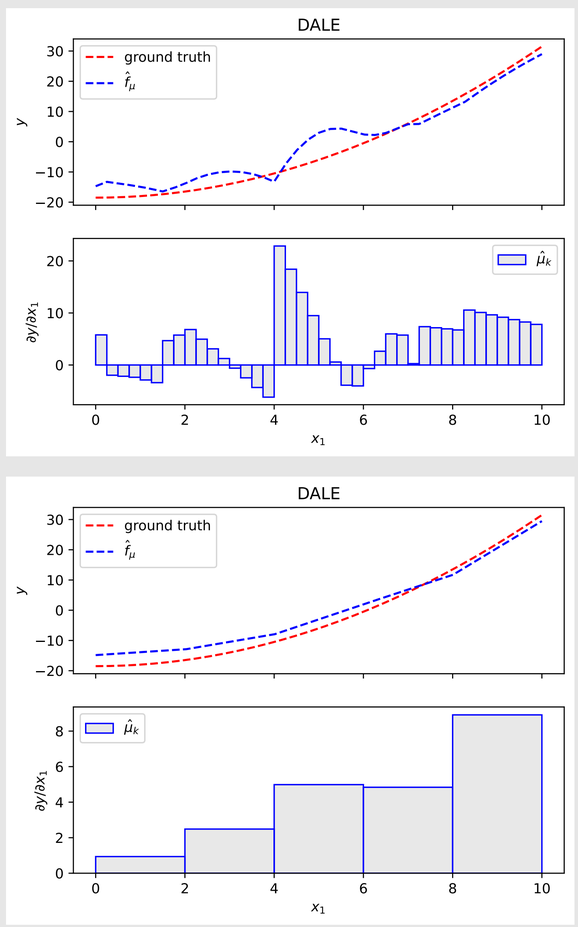
$$f(x_s) = \Delta x \sum_{k}^{k_x} \underbrace{\frac{1}{|\mathcal{S}_k|} \sum_{i:\mathbf{x}^i \in \mathcal{S}_k} \underbrace{[\frac{\partial f}{\partial x_s}(x_s^i, \boldsymbol{x_c^i})]}_{\textbf{point effect}}}_{\text{bin effect}}$$

DALE approximation addresses these issues. The main difference is the use of automatic differentiation, instead of evaluating at the bin limits.

DALE saves from OOD



Consider the following case; (a) we have limited samples (b) high variance and (c) the black-box function changes abruptply outside the data manifold. For example, $f(x_1, x_2, x_3) = x_1x_2 + x_1x_3 \pm g(x)$, with $x_1 \in [0, 10]$, $x_2 = x_1 + \epsilon$ and $x_3 \sim \mathcal{N}(0, \sigma^2)$. The term x_1x_3 makes estimations from limited samples noisy, so we need to grow the bins larger (more $\frac{\text{points}}{\text{bin}}$). But as we grow bins, ALE creates OOD samples,



DALE is much more efficient

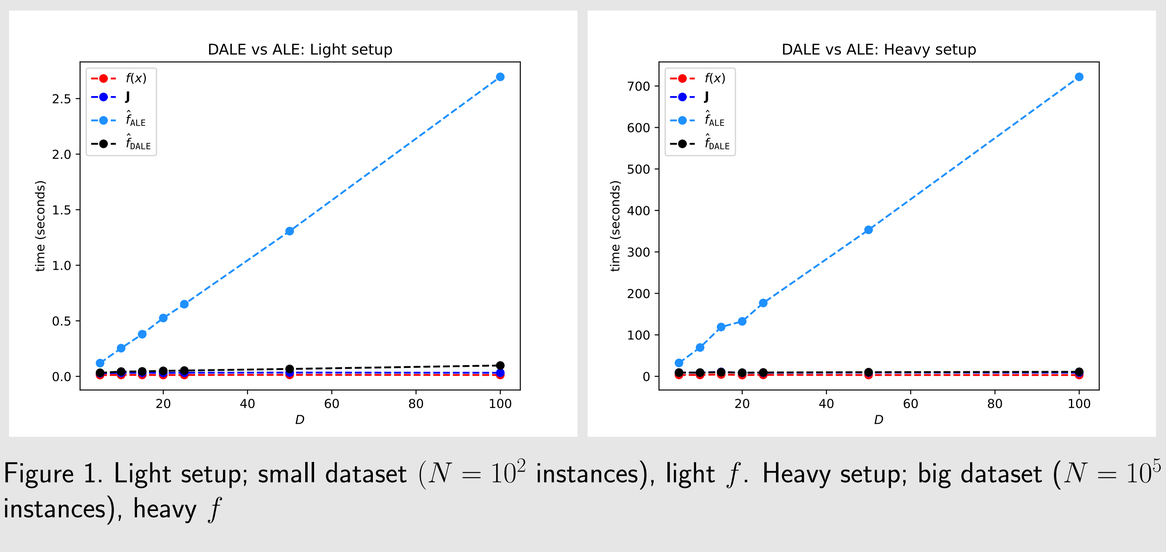


Figure 1. Light setup; small dataset ($N = 10^2$ instances), light f. Heavy setup; big dataset ($N = 10^5$ instances), heavy f

Conclusion

In case you work with a differentiable model, as in Deep Learning, use DALE to:

- compute feature effect wrt all features in near the same time as to computing the
- have the versatility to compute many different bin sizes, in near zero computational cost
- be sure that your estimation is based on on-distribution samples, irrespectively of the bin size

References

Apley, D. W. and J. Zhu (2020). "Visualizing the effects of predictor variables in black box supervised learning models". In: *Journal of the Royal Statistical Society. Series B: Statistical Methodology* 82.4, pp. 1059–1086. ISSN: 14679868. DOI: 10.1111/rssb.12377. arXiv: 1612.08468.