

Hannah Blocher, Georg Schollmeyer, Christoph Jansen, Malte Nalenz
Ludwig–Maximilians–Universität München

Depth Functions for Partial Orders **with a Descriptive Analysis of Machine Learning Algorithms**

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Working Group



Working Group *Foundations of Statistics and their Applications* of Prof. Dr. Thomas Augustin.

(From left to right: Malte Nalenz, Dominik Kreiß (back), Hannah Blocher (front), Christoph Jansen, Thomas Augustin, Julian Rodemann, Gilbert Kiprotich, Georg Schollmeyer)

Depth Functions for Partial Orders

with a Descriptive Analysis of Machine Learning Algorithms

Depth Function

Depth Functions measure **centrality** and **outlingless** of a data point with respect to a data cloud or an underlying distribution.

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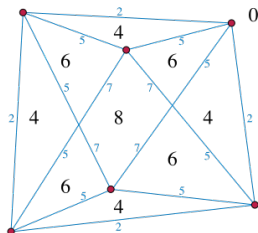


Figure: Simplicial Depth

(see https://en.wikipedia.org/wiki/Simplicial_depth, visited: 20.10.21)

Depth Function

Depth Functions measure **centrality** and **outlingless** of a data point with respect to a data cloud or an underlying distribution.

Idea: Adaptation of the simplicial depth to the set of partial orders

Approach: The representation of the simplicial depth via the convex closure system

Result: *union-free generic (ufg) depth function*

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Comparison of Machine Learning Algorithms

- Data Sets: 80 classification problems from OpenML.
 - ML Algorithms: Random Forests (RF), Decision Tree (CART), Logistic regression (LR), L1-penalized logistic regression (Lasso) and k-nearest neighbours(KNN).
 - Performance Measures: area under the curve, F-score, predictive accuracy and Brier score.
- ⇒ We obtain 80 posets

Comparison of Machine Learning Algorithms

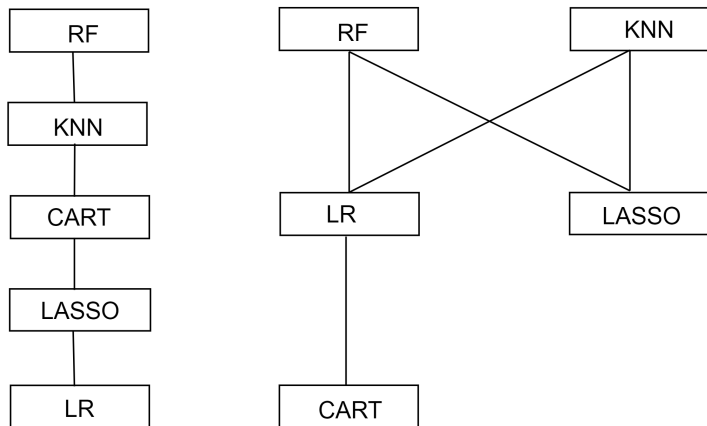


Figure: Example of two posets obtained by comparing five ml algorithms based on four performance measures. Each poset describes the performance based on one data set.

Minimal and Maximal Depth Value

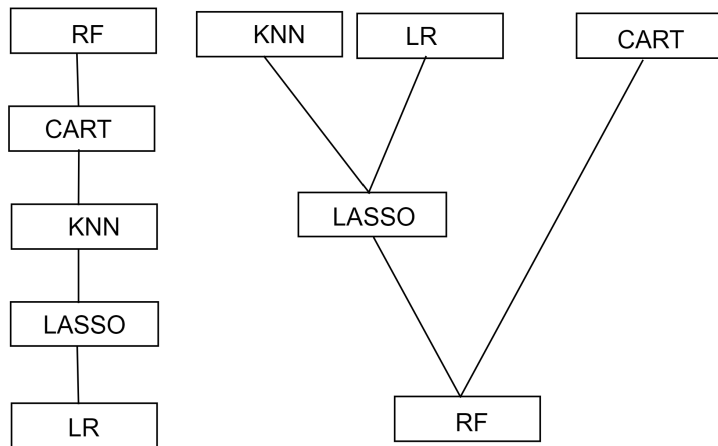


Figure: Observed poset with maximal (left) and minimal (right) ufg depth.



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Department of Statistics, Ludwig-Maximilians-Universität München

hannah.blocher@stat.uni-muenchen.de

General Situation

- A sample of partial orders (e.g. compare the performance of ml algorithms on a fixed data set w.r.t. multiple performance measures at once).
- Each partial order is indeed a precise observation. Thus, items are allowed to be incomparable.
- Partial orders on a special case of non-standard data.

Contribution

- Introducing the *alg* depth function (give a center-outward order) to obtain a description of the distribution of partial orders (P) based on a sample.
- Explicitly addressing incomparability in the data description.

Idea: Adaptation of the Simplicial Depth

Depth functions measure the centrality and outlyingness of a data point with respect to a data cloud or an underlying distribution.

Simplicial Depth

Union-Free Generic Depth

Define the Closure Operator System

$$\gamma_{\text{SD}}: 2^{\mathcal{A}} \rightarrow 2^{\mathcal{A}}, A \mapsto \left\{ a \in \mathcal{A} \mid \exists \{a_1, \dots, a_n\} \subseteq A \text{ with } a_i \in A \right. \\ \left. \wedge \{a_1, \dots, a_n\} \subseteq \mathcal{A} \wedge a = \bigwedge_{i=1}^n a_i \wedge a, a_i \in N \right\}$$

$$\gamma: 2^{\mathcal{A}} \rightarrow 2^{\mathcal{A}}, P \mapsto \left\{ a \in \mathcal{A} \mid \bigcap_{a \in P} \beta \subseteq \bigcup_{a \in P} \alpha \right\}$$



Reduce the Input Set (It is Still Sufficient to Describe the Closure Operator)

$$\gamma' := \{[A, B, C] \subseteq \mathcal{A}\}$$

$$\gamma' := \{P \subseteq \mathcal{P} \mid \text{Condition (C1) and (C2) hold}\}$$



- with
- (C1) $P \subseteq \mathcal{P}$
 - (C2) There does not exist a family $\{A_i\}_{i=1}^n$ such that for all $i \in \{1, \dots, n\}$: $A_i \subseteq P$ and $\bigcup_{i=1}^n \gamma(A_i) = \gamma(P)$.

Define the Depth Function (M is a Set of Probability Measures)

$$D: \mathcal{A}^n \times \mathcal{M} \rightarrow [0, 1] \\ (x, \mu) \mapsto \mu(\gamma_{\text{SD}}(\{x_1, \dots, x_n\}))$$

$$D: \mathcal{P} \times \mathcal{M} \rightarrow [0, 1] \\ (P, \mu) \mapsto \int \int_{\mathcal{A}^n} \mathbb{1}_{\gamma(P)} \left(\bigwedge_{i=1}^n x_i \right) \mu^{\otimes n}(dx) = \int \mu^{\otimes n}(\gamma(P)) = \mu^{\otimes n}(\gamma(P))$$

Comparison of Machine Learning Algorithms

For each data set we compare a set of ml algorithms based on multi-dimensional performance measures. This leads to a partial order for every data set.

- Data Set: 80 classification problems from OpenML.
- ML Algorithms: Random Forests (RF), Decision Tree (CART), Logistic regression (LR), L1 penalized logistic regression (Lasso) and k-nearest neighbors (KNN).
- Performance Measures: avg. under the curve, F-score, predictive accuracy and Brier score.



Figure 1: Observed pair with maximal (alg) and minimal (alg) depth.



Figure 2: Observed pair with maximal (alg) and minimal (alg) depth.

Outlook

- Other types of non-standard data.
- Statistical inference.
- Other ML problems and criteria.
- ...

References

- Blocher, Schollmeyer, Jansen, Nalenz (2023): Depth Functions for Partial Orders with a Descriptive Analysis of Machine Learning Algorithms. Preprint on arXiv:2310.14111.
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