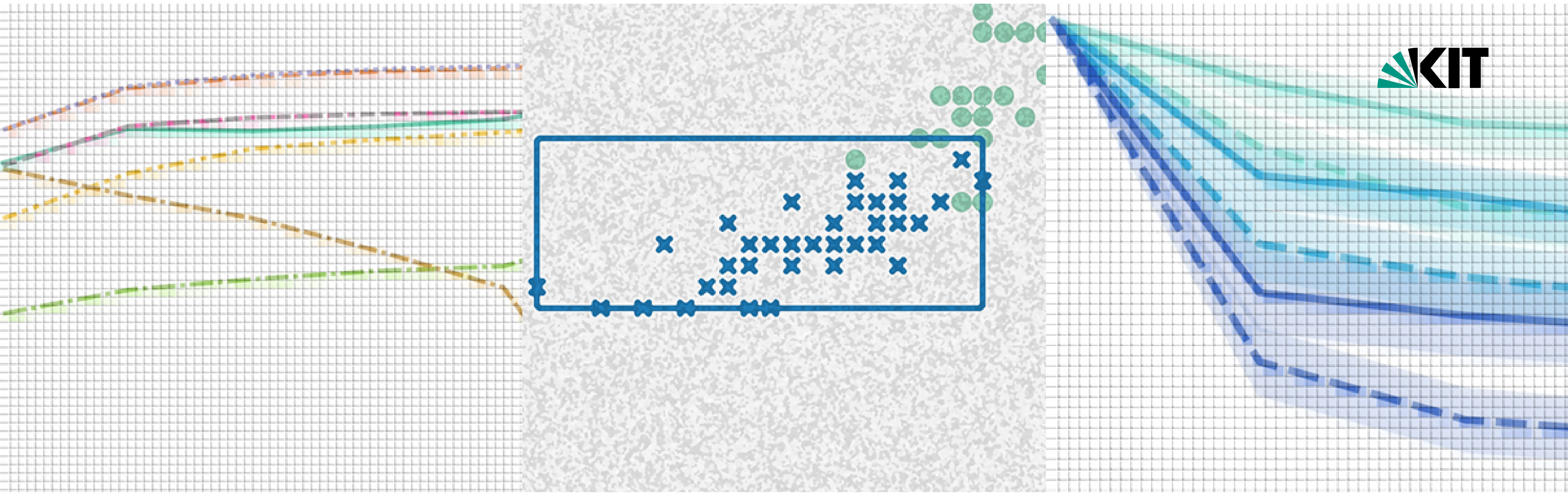

Subgroup Discovery with Small and Alternative Feature Sets

SIGMOD 2025 | Berlin

Jakob Bach (jakob.bach@kit.edu) | June 24, 2025

Subgroup Discovery

- **Subgroup discovery:** "Identifying descriptions of subsets of a dataset that show an interesting behavior" [1]
  - Language for descriptions typically simple
  - 'Interesting' according to some objective function

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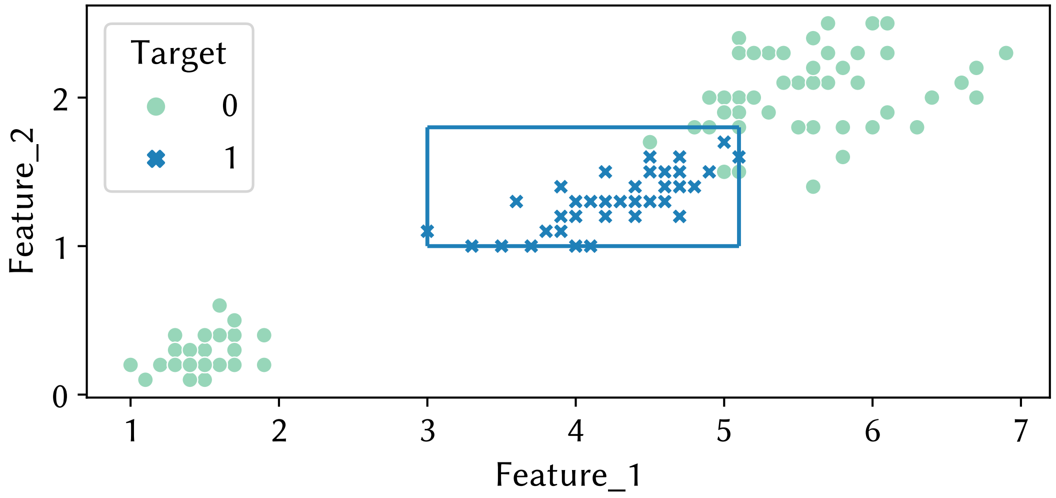
- **Our scope:** Binary classification with real-valued features
  - Tabular dataset $X \in \mathbb{R}^{m \times n}$ (data objects $\times$ features)
  - Prediction target $y \in \{0, 1\}^m$ (‘interesting’/‘positive’ = 1)
  - Subgroup description: Hyperrectangle
  - Subgroup quality: Weighted Relative Accuracy
    - $\text{WRAcc} = \frac{m_b}{m} \cdot \left(\frac{m_b^+}{m_b} - \frac{m^+}{m} \right)$ [22]
    - $+ \leftrightarrow$ positive data object, $b \leftrightarrow$ in subgroup (box)



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- **Contributions:**
  - Formalize subgroup discovery as an SMT (Satisfiability Modulo Theories) optimization problem
  - Formalize two constraint types:
    - Feature-cardinality constraints
    - Alternative subgroup descriptions
  - Analyze computational complexity and show $\mathcal{NP}$-hardness
  - Comprehensive experiments

Formalization – Basic Problem

$$lb, ub \in \{\mathbb{R} \cup \{-\infty, +\infty\}\}^n \qquad \text{(Variables: lower/upper bounds of subgroup)}$$

Formalization – Basic Problem

$$\forall j \in \{1, \ldots, n\} \quad lb_j \leq ub_j \quad \text{(Constraint: relationship between bounds)}$$

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Formalization – Basic Problem

$$
\begin{array}{lll}
\forall i \in \{1, \dots, m\} & b_i \leftrightarrow \bigwedge\limits_{j \in \{1, \dots, n\}} \left((X_{ij} \geq lb_j) \land (X_{ij} \leq ub_j) \right) & \text{(i-th data object in subgroup?)} \\
\forall j \in \{1, \dots, n\} & lb_j \leq ub_j & \text{(Constraint: relationship between bounds)} \\
 & b \in \{0, 1\}^m & \text{(Auxiliary variables: subgroup membership)} \\
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Formalization – Basic Problem

s.t.:

$$m_b := \sum_{i=1}^{m} b_i \quad \text{and} \quad m_b^+ := \sum_{\substack{i \in \{1,\dots,m\} \\ y_i = 1}} b_i \qquad \text{(Number of data objects in subgroup)}$$

$$\forall i \in \{1, \dots, m\} \quad b_i \leftrightarrow \bigwedge_{j \in \{1,\dots,n\}} \left((X_{ij} \geq lb_j) \land (X_{ij} \leq ub_j) \right) \qquad \text{(i-th data object in subgroup?)}$$

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\begin{array}{llll}
\max & & Q_{\text{WRAcc}} = \frac{m_b^+}{m} - \frac{m_b \cdot m^+}{m^2} & \text{(Objective: subgroup quality)} \\
\text{s.t.:} & & m_b := \sum_{i=1}^{m} b_i \quad \text{and} \quad m_b^+ := \sum_{\substack{i \in \{1,\dots,m\} \\ y_i = 1}} b_i & \text{(Number of data objects in subgroup)} \\
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\forall j \in \{1, \dots, n\}: \quad & s_j \leftrightarrow \left(s_j^{\text{lb}} \lor s_j^{\text{ub}} \right)
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$$\sum_{j=1}^{n} s_j \leq k$$

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$$\text{sim}_{\text{nHamm}}(b^{(a)}, b^{(0)}) = \frac{1}{m} \cdot \sum_{i=1}^{m} \left(b_i^{(a)} \leftrightarrow b_i^{(0)} \right) = \frac{1}{m} \cdot \Bigg(\sum_{\substack{i \in \{1,\dots,m\} \\ b_i^{(0)}=1}} b_i^{(a)} + \sum_{\substack{i \in \{1,\dots,m\} \\ b_i^{(0)}=0}} \neg b_i^{(a)} \Bigg)$$

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- **Chosen dissimilarity constraints:** From each existing feature set, deselect at least $\tau_{\text{abs}} \in \mathbb{N}$ (but $\leq k$) features

$$\forall l \in \{0, \dots, a-1\}: \ \text{dis}_{\text{des}}(s^{(a)}, s^{(l)}) = \sum_{\substack{j \in \{1,\dots,n\} \\ s_j^{(l)}=1}} \neg s_j^{(a)} \geq \min\left(\tau_{\text{abs}},\ k^{(l)}\right)$$

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  - Solver timeouts: {1 s, 2 s, 4 s, . . . , 2048 s}
  - Feature-cardinality constraints: $k \in \{1, 2, 3, 4, 5\}$, 'no' (unconstrained)
  - Alternative subgroup descriptions: $k = 3$ features, $a = 5$ alternatives, and dissimilarity threshold $\tau_{\text{abs}} \in \{1, 2, 3\}$

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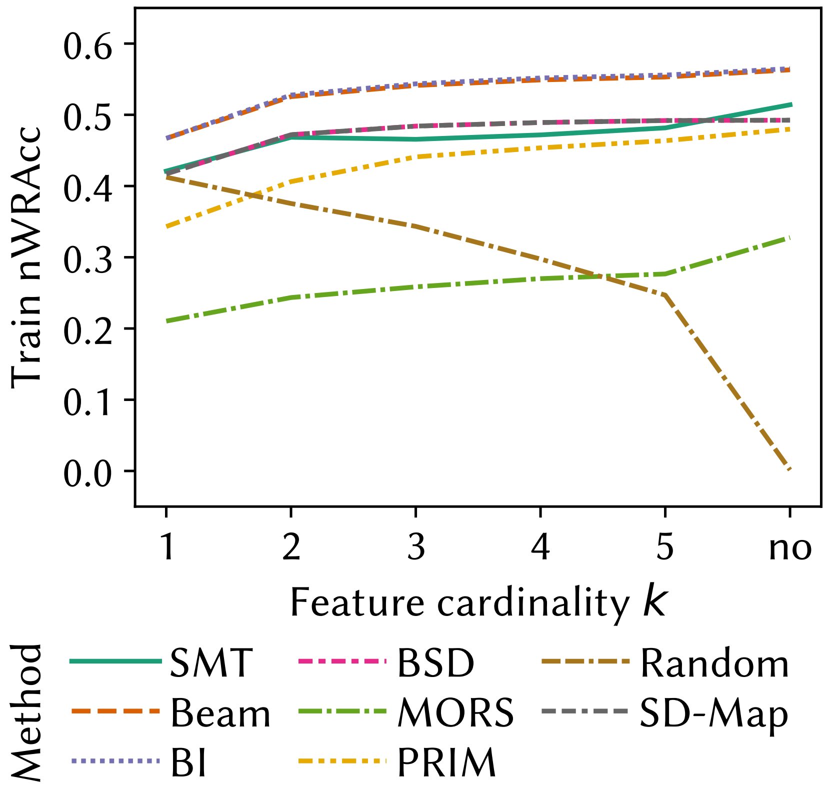
- **Evaluation metrics:**
  - Subgroup quality (nWRAcc [22, 29])
  - Runtime
  - For alternatives: Similarity [12] (Normalized Hamming and Jaccard)

Results – Feature-Cardinality Constraints



(a) All 27 datasets.

Subgroup quality of original subgroups.

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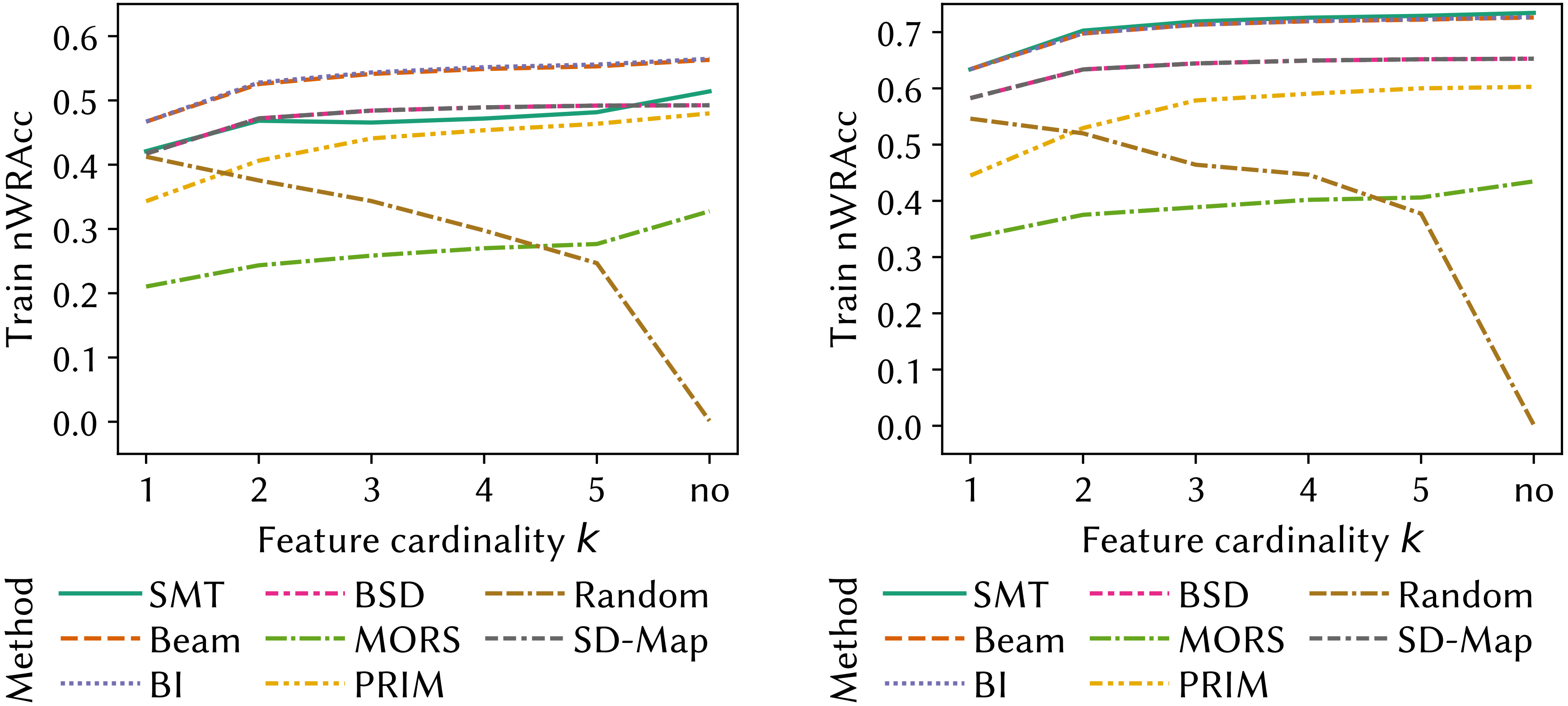

(a) All 27 datasets.

(b) 13 datasets without *SMT* timeouts.

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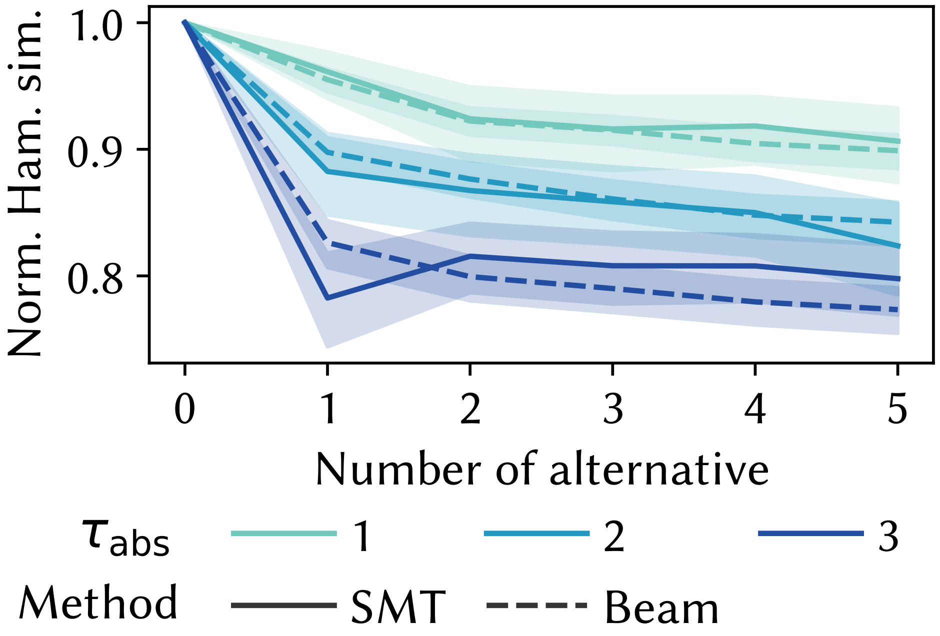
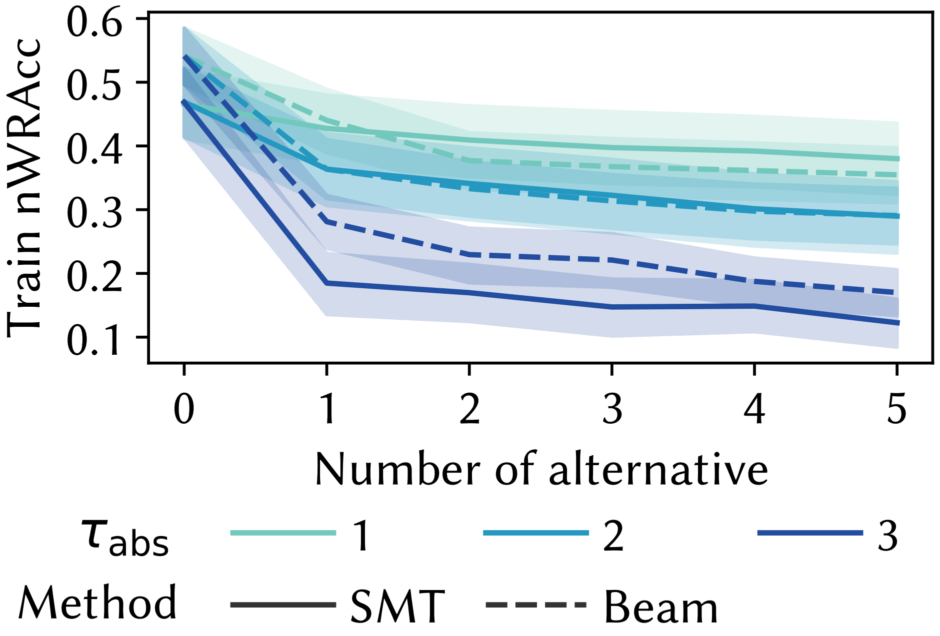


(a) Subgroup similarity.



(b) Subgroup quality.

Similarity and quality of alternative subgroup descriptions.

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  - Different subgroup descriptions (used features) may capture similar subgroup (set of data objects)
- **Resources:**
  - Paper [5] (longer arXiv version [6])
  - Code [3] (including Python package `csd` with subgroup-discovery methods)
  - Experimental data [4]

Appendix

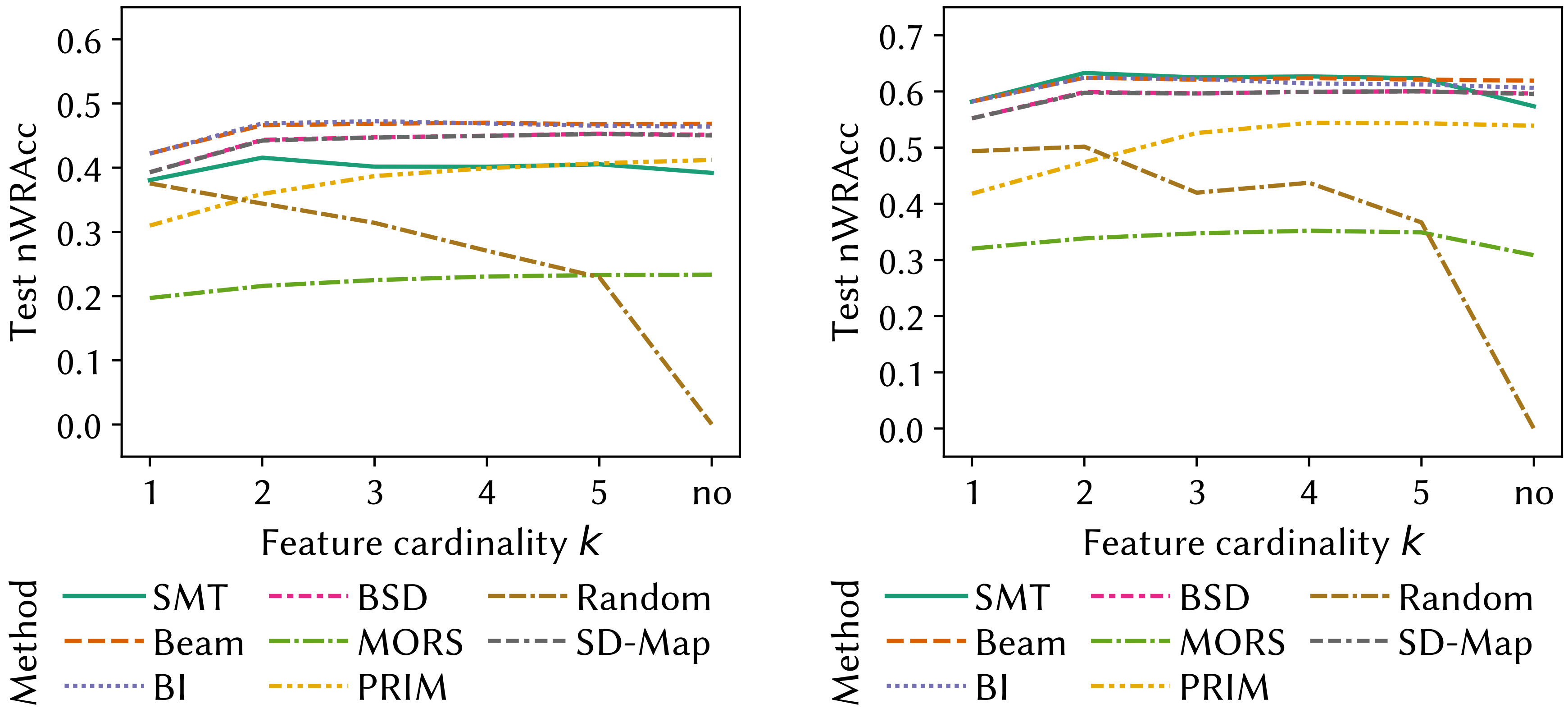
Related Work

- Existing subgroup-discovery methods [1, 18, 19, 34] typically algorithmic (exhaustive or heuristic)
- Few white-box formulations of (other) variants of subgroup discovery [10, 14, 17, 21, 26]
- Concept of feature cardinality well-established [19, 30], but empirical studies varying it [15, 24, 30, 32] are limited
- Concept of alternative subgroups well-established [1, 7, 11, 23, 27], but alternative descriptions [9, 16, 23, 25] less

Computational Complexity

- Subgroup discovery with a feature-cardinality constraint is $\mathcal{NP}$-complete
- **Proof:** Reduction from SET COVERING [20]
  - Set-covering problem: Given set of elements $E = \{e_1, \dots, e_m\}$, set of sets $\mathbb{S} = \{S_1, \dots, S_n\}$ with $E = \bigcup_{S \in \mathbb{S}} S$, and a cardinality $k \in \mathbb{N}$, does subset $\mathbb{C} \subseteq \mathbb{S}$ with $|\mathbb{C}| \leq k$ and $E = \bigcup_{S \in \mathbb{C}} S$ exist?
  - Perfect-subgroup discovery: Find subgroup containing all positive data objects ($y_i = 1$) and zero negatives ($y_i = 0$)
  - Problem transformation:
    - Dataset $X \in \{0, 1\}^{(m+1) \times n}$ with $X_{ij} := (e_i \in S_j)$
    - Data object $m + 1$ represents an element not contained in any set, i.e., $X_{(m+1)j} = 0$ for all $j \in \{1, \dots, n\}$
    - Prediction target $y \in \{0, 1\}^{m+1}$ with $y_{m+1} = 1$ and $y_i = 0$ otherwise
  - Perfect subgroup only contains data object $m + 1$ and uses $lb_j = ub_j = 0$ conditions for selected features
  - Other data objects have value 1 for at least one selected feature $\rightarrow$ each element is in a selected set
  - I.e., algorithm for perfect-subgroup discovery also solves SET COVERING
  - Optimizing subgroup quality typically at least as hard as finding perfect subgroup
- Finding alternative subgroup descriptions with a feature-cardinality constraint is $\mathcal{NP}$-complete as well

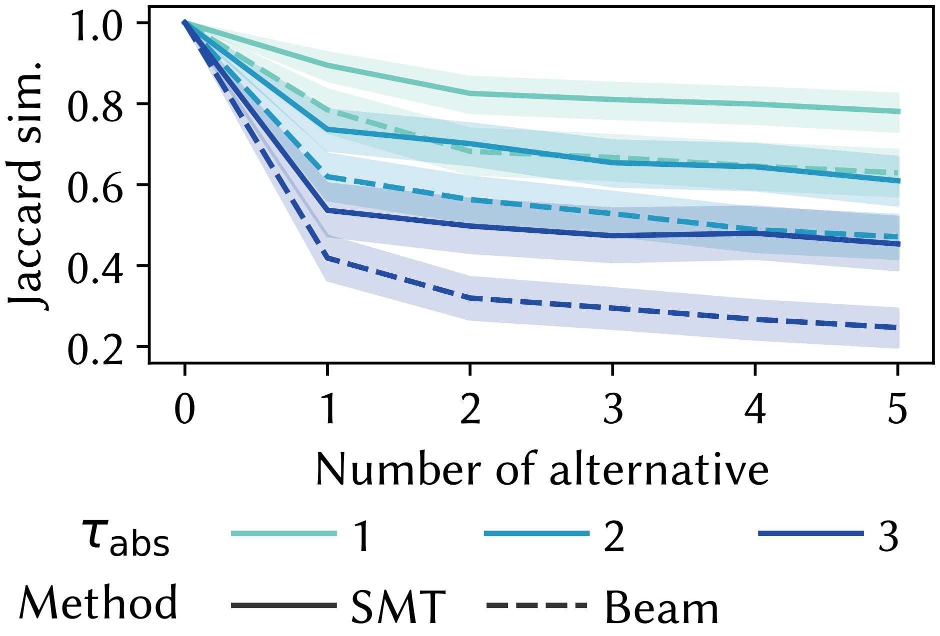
More Results – Feature-Cardinality Constraints



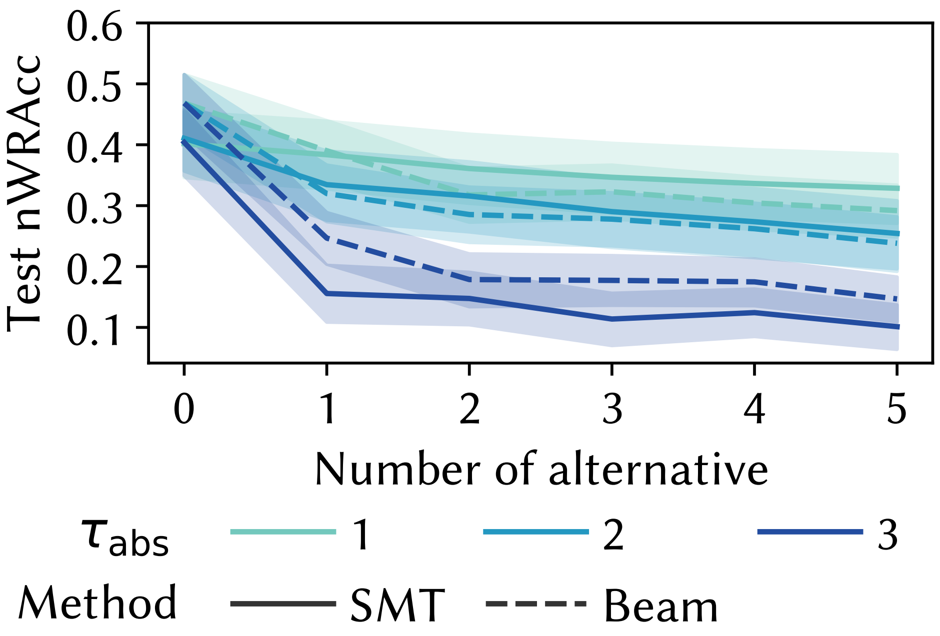
(a) All 27 datasets. (b) 13 datasets without *SMT* timeouts.

Subgroup quality of original subgroups on the test set.

More Results – Alternative Subgroup Descriptions



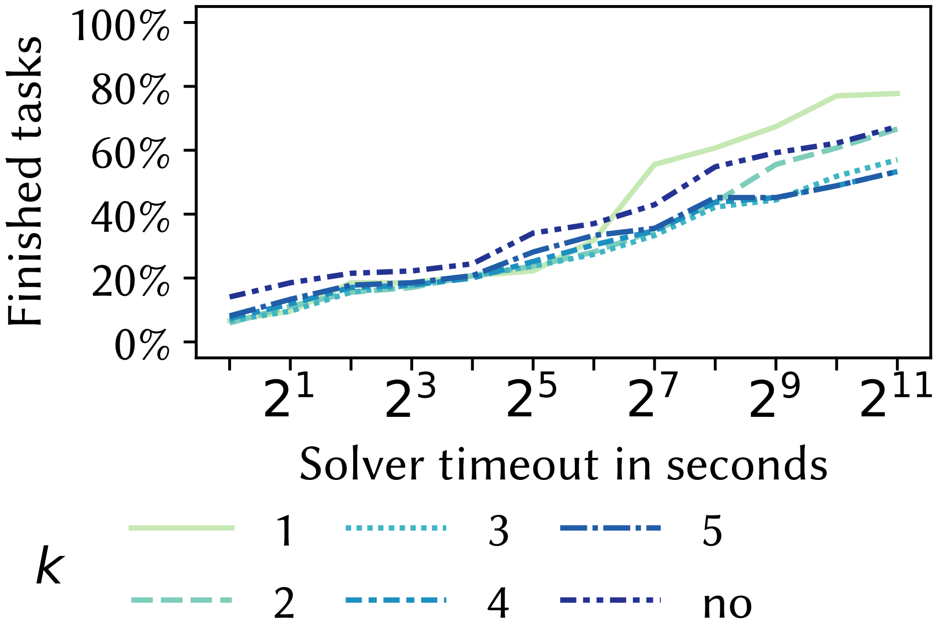
(a) Subgroup similarity (Jaccard).



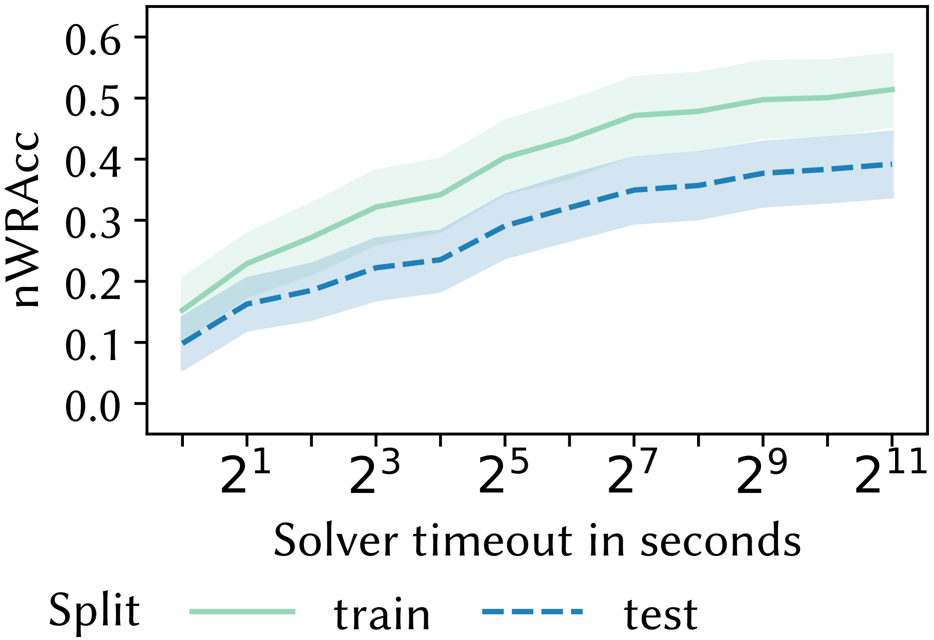
(b) Subgroup quality on the test set.

Similarity and quality of alternative subgroup descriptions.

More Results – Solver Timeouts



(a) Frequency of finished *SMT* tasks.



(b) Subgroup quality.

Impact of solver timeouts for *SMT* as the subgroup-discovery method.

More Results – Runtime

Mean runtime (in sec.) for searching original subgroups.

k	1	2	3	4	5	no
BI	7.8	11.7	14.2	16.7	18.7	35.0
BSD	0.9	0.9	0.9	2.7	29.5	55.7
Beam	6.8	10.1	12.8	14.6	16.1	30.5
MORS	0.0	0.0	0.0	0.0	0.0	0.0
PRIM	0.1	0.2	0.3	0.3	0.5	1.3
Random	0.6	0.6	0.6	0.7	0.7	0.9
SD-Map	2.3	3.3	9.6	54.0	345.2	367.4
SMT	648.2	911.3	1091.7	1113.4	1117.4	849.0

Mean runtime (in sec.) for searching alternative subgroup descriptions.

Method	τ_{abs}	Number of alternative					
		0	1	2	3	4	5
Beam	1	12.8	8.0	7.6	7.3	7.3	7.3
	2	12.8	7.7	7.4	7.2	7.0	6.8
	3	12.8	5.8	5.1	4.7	4.1	3.5
SMT	1	1091.7	166.0	221.5	239.6	258.1	277.9
	2	1105.2	377.5	463.5	537.5	599.4	658.3
	3	1107.4	869.1	670.8	597.6	588.1	557.6

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