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Leveraging Constraints for User-Centric Feature Selection

PhD Defense

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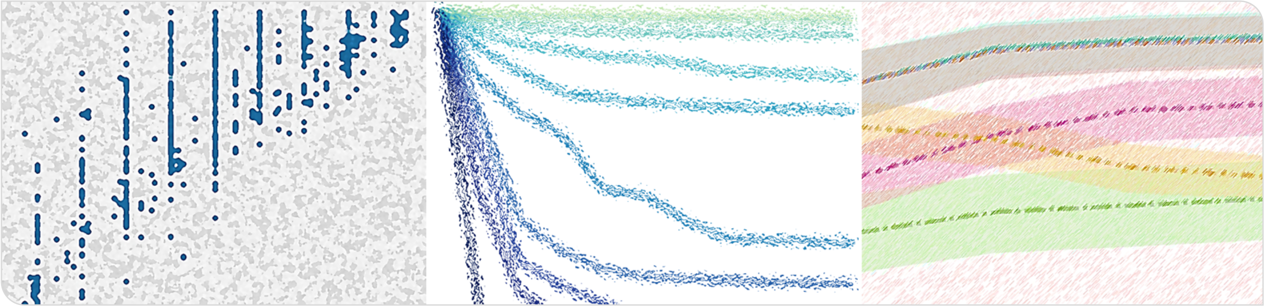

Background

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Definition (Feature selection)

Given a dataset $X \in \mathbb{R}^{m \times n}$ with prediction target $y \in Y^m$ (e.g., $Y = \mathbb{R}$ or $Y = \{0, 1\}$),
feature selection is the problem of making feature-selection decisions $s \in \{0, 1\}^n$
that maximize a given notion of feature-set quality $Q(s, X, y)$.
Typically, select a fixed number of features $k \in \mathbb{N}$, i.e., $\sum_{j=1}^{n} s_j = k$.

- Reasons for feature selection [13, 34]:
  - Increase interpretability of predictions
  - Reduce computational requirements of machine learning (CPU, memory, storage, power consumption)
  - Improve prediction performance

Feat_1	Feat_2	...	Feat_n	Target
X_{11}	X_{12}	...	X_{1n}	y_1
X_{21}	X_{22}	...	X_{2n}	y_2
...	...	...	...	...
X_{m1}	X_{m2}	...	X_{mn}	y_m

Motivation and Our Approach

- Main limitations of most existing feature-selection methods:
  - Do not consider domain knowledge
  - Return only one feature set, no alternatives
- Central idea of dissertation: Make feature selection more user-centric via constraints
  - Still optimize feature-set quality but restrict valid feature selections
  - Formulate as white-box optimization problem and use solver

Example (A feature-selection constraint)

$(\neg s_1 \land \neg s_2 \land \neg s_3) \lor (s_1 \land s_2 \land s_3) \leftrightarrow$ “Select none or all of Features 1, 2, and 3.”

- Benefits of our approach:
  - Declarative
  - Allows combining constraints
  - Orthogonal to choice of feature-selection method

Our Contributions

- (C1) Evaluating the impact of constraints [7]
  - Formalize constrained feature selection
  - Conduct domain-independent study on impact of constraints
- (C2) Using constraints to formulate scientific hypotheses [7]
  - Conduct domain-specific study on impact of constraints
- (C3) Using constraints for alternative feature sets [3, 6]
  - Formalize alternative feature selection
  - Discuss integrating constraints
  - Analyze time complexity
  - Propose heuristic search methods
  - Conduct experimental study
- (C4) Using constraints for feature selection in subgroup discovery [4, 5]
  - Formalize subgroup discovery as SMT optimization problem
  - Formalize two constraint types
  - Discuss integrating constraints
  - Analyze time complexity
  - Conduct experimental study
- Reproducibility:
  - All experimental data available on RADAR4KIT
  - Three GitHub repositories [a, b, c]
  - Three Python packages: `alfese`, `cffs`, `csd`

(C1) Evaluating the Impacts of Constraints – Approach

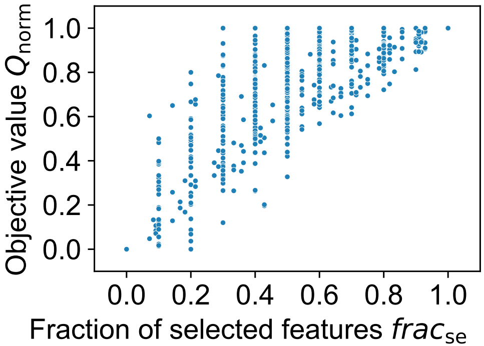
- Systematic study on impact of constraints on feature-selection results
  - Metrics for constraints, e.g., fraction of valid feature sets
  - Metrics for results, e.g., feature-set quality

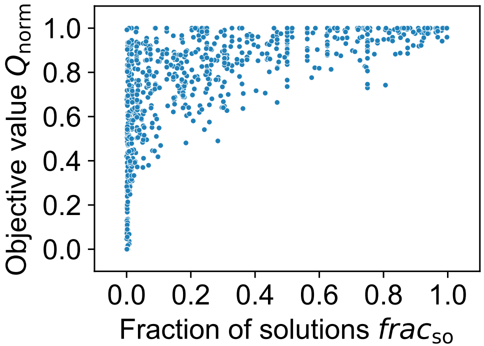
- Experimental design:
  - 35 regression datasets from *OpenML* [53]
  - Linear objective: $Q(s, X, y) = \sum_{j=1}^{n} q(X_{\cdot j}, y) \cdot s_j$ (using mutual information [29] as $q(\cdot)$)
  - Generate random constraints for ten constraint types with 1000 repetitions
  - *Z3* [10, 16] (an SMT solver) as optimizer

Examples (Constraint types)

- Single-XOR$(s_{j_1}, s_{j_2}) = s_{j_1} \oplus s_{j_2} = (s_{j_1} \land \neg s_{j_2}) \lor (\neg s_{j_1} \land s_{j_2})$
- Group-NAND$(\{s_{j_1}, \dots, s_{j_{n'}}\}) = \neg(s_{j_1} \land s_{j_2} \land \dots \land s_{j_{n'}}) = \sum_{l=1}^{n'} s_{j_l} \leq n' - 1$

(C1) Evaluating the Impacts of Constraints – Results





$$frac_{\text{se}} = \frac{\sum_{j=1}^{n} s_j}{n} \quad \Big| \quad Q_{\text{norm}} = \frac{\sum_{j=1}^{n} s_j \cdot q(X_{\cdot j}, y)}{\sum_{j=1}^{n} q(X_{\cdot j}, y)} \quad \Big| \quad frac_{\text{so}} = \frac{\sum_{s \in \{0,1\}^n} \min_{c \in C} c(s)}{2^n}$$

(C3) Alternative Feature Selection – Approach

- Idea: Find feature sets optimizing feature-set quality while differing from each other
  - Domain-independent constraint type
  - Orthogonal to choice of feature-selection method
  - Number of alternatives $a \in \mathbb{N}_0$ and feature-set dissimilarity threshold $\tau \in [0, 1]$ as user parameters
  - Sequential or simultaneous search

Sequential-search problem

$$\max_{s} \quad Q(s, X, y)$$
$$\text{subject to:} \quad \forall F' \in \mathbb{F}: \; d(F_s, F') \geq \tau$$

Simultaneous-search problem

$$\max_{s^{(0)},\dots,s^{(a)}} \quad \underset{l \in \{0,\dots,a\}}{\operatorname{agg}} \quad Q(s^{(l)}, X, y)$$
$$\text{subject to:} \quad \forall l_1, l_2 \in \{0, \dots, a\}, \; l_1 \neq l_2: \; d(F_{s^{(l_1)}}, F_{s^{(l_2)}}) \geq \tau$$

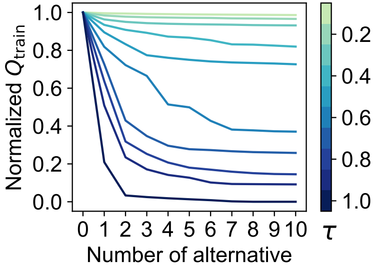
- Chosen dissimilarity measure: $d_{\text{Dice}}(F', F'') = 1 - \frac{2 \cdot |F' \cap F''|}{|F'| + |F''|} = 1 - \frac{2 \cdot \sum_{j=1}^{n} s'_j \cdot s''_j}{\sum_{j=1}^{n} s'_j + \sum_{j=1}^{n} s''_j}$

(C3) Alternative Feature Selection – Complexity

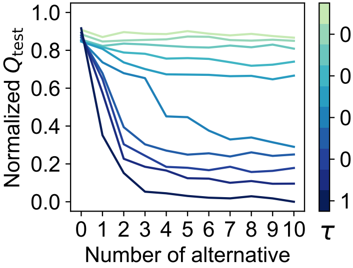
- Alternative feature selection is $\mathcal{NP}$-complete in scenario with:
  - Simultaneous search with minimum as aggregation operator agg($\cdot$)
  - Linear notion of feature-set quality: $Q(s, X, y) = \sum_{j=1}^{n} q_j \cdot s_j$
  - No feature-set overlap ($\tau = 1$)
  - Complete partitioning (each feature part of exactly one feature set)
- Proof: Known as MULTI-WAY NUMBER PARTITIONING [28] or MULTIPROCESSOR SCHEDULING [22] □

- Further complexity-related contributions and results:
  - Prove $\mathcal{NP}$-hardness for (1) incomplete partitioning and (2) feature-set overlap
  - Prove polynomial runtime for sum-aggregation and sequential search with remaining conditions from above
  - Develop two heuristic search methods with approximation guarantee

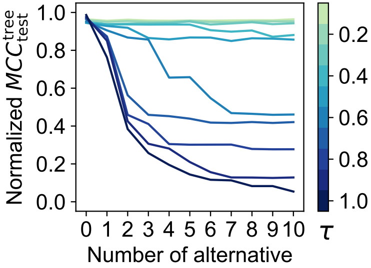
(C3) Alternative Feature Selection – Empirical Results



(a) Training-set objective value.



(b) Test-set objective value.



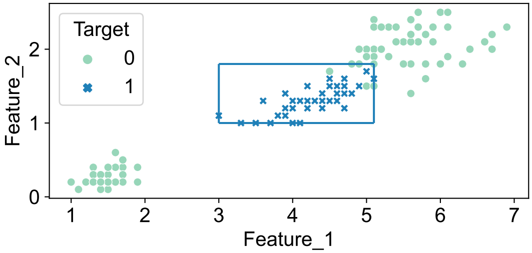
(c) Test-set prediction performance.

Mean of feature-set quality, over the number of alternatives and dissimilarity threshold τ, by evaluation metric.

(C4) Constrained Subgroup Discovery – Approach

- Subgroup discovery: “Identifying descriptions of subsets of a dataset that show an interesting behavior” [1]

- 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 quality: Weighted Relative Accuracy
    - WRAcc $= \frac{m_b}{m} \cdot \left(\frac{m_b^+}{m_b} - \frac{m^+}{m} \right)$ [31]
    - $+ \leftrightarrow$ positive data object, $b \leftrightarrow$ in subgroup (box)



- Our goal: Improve interpretability with constraints
  - Limit number of used features
  - Find alternative subgroup descriptions

(C4) Subgroup Discovery – Formalization: Basic Problem

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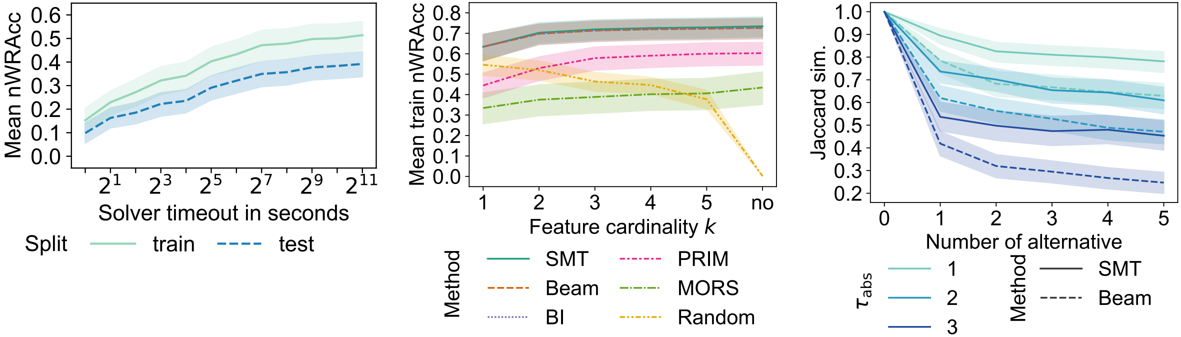
$$
\begin{array}{lll}
\max & Q_{\text{WRAcc}} = \frac{m_b^+}{m} - \frac{m_b \cdot m^+}{m^2} & \text{(Objective: subgroup quality)} \\
\text{s.t.:} & m_b := \sum_{i=1}^{m} b_i \quad \text{and} \quad m_b^+ := \sum_{\substack{i \in \{1,\dots,m\} \\ y_i = 1}} b_i & \text{(Num of data objects in subgroup)} \\
\forall i \in \{1, \dots, m\} & b_i \leftrightarrow \bigwedge_{j \in \{1,\dots,n\}} \left((X_{ij} \geq lb_j) \land (X_{ij} \leq ub_j) \right) & \text{(i-th data object in subgroup?)} \\
\forall j \in \{1, \dots, n\} & lb_j \leq ub_j & \text{(Constraint: relationship between bounds)} \\
 & b \in \{0, 1\}^m & \text{(Auxiliary variables: subgroup membership)} \\
 & lb, ub \in \{\mathbb{R} \cup \{-\infty, +\infty\}\}^n & \text{(Variables: lower/upper bounds of subgroup)}
\end{array}
$$

(C4) Subgroup Discovery – Formalization: Cardinality

- Concept: Limit number of features used (= selected) in subgroup description to $k \in \mathbb{N}$
- Formally: Limit number of features whose bounds exclude at least one data object from subgroup

$$
\begin{aligned}
\forall j \in \{1, \ldots, n\}: \quad & s_j^{\text{lb}} \leftrightarrow \left(lb_j > \min_{i \in \{1, \ldots, m\}} X_{ij} \right) \\
\forall j \in \{1, \ldots, n\}: \quad & s_j^{\text{ub}} \leftrightarrow \left(ub_j < \max_{i \in \{1, \ldots, m\}} X_{ij} \right) \\
\forall j \in \{1, \ldots, n\}: \quad & s_j \leftrightarrow \left(s_j^{\text{lb}} \lor s_j^{\text{ub}} \right) \\
& \sum_{j=1}^{n} s_j \leq k \\
& s, s^{\text{lb}}, s^{\text{ub}} \in \{0, 1\}^n
\end{aligned}
$$

(C4) Constrained Subgroup Discovery – Empirical Results



Mean subgroup quality over solver timeouts for *SMT* search.

Mean training-set subgroup quality over feature-cardinality threshold k.

Mean similarity of alternative subgroup descriptions.

Conclusions

- Research gaps – Most existing methods for feature selection:
  - Do not consider domain knowledge
  - Return only one solution, no alternatives
- Approach: Address both research gaps with constraints on selected feature sets
- Core contributions:
  - (C1) Evaluating the impact of constraints: Bach et al. (2022) [7]
  - (C2) Using constraints to formulate scientific hypotheses: Bach et al. (2022) [7]
  - (C3) Using constraints for alternative feature sets: Bach (2024) [3], Bach and Böhm (2024) [6]
  - (C4) Using constraints for feature selection in subgroup discovery: Bach (2025) [4], Bach (2024) [5]
- All code and data available online

Appendix

Details of Our Underlying Publications

- Constrained feature selection (C1 and C2):
  - Jakob Bach et al. “An Empirical Evaluation of Constrained Feature Selection”. In: *SN Comput. Sci.* 3.6 (2022). DOI: 10.1007/s42979-022-01338-z
- Alternative feature selection (C3):
  - Jakob Bach. *Finding Optimal Diverse Feature Sets with Alternative Feature Selection*. arXiv:2307.11607v2 [cs.LG]. 2024. DOI: 10.48550/arXiv.2307.11607
  - Jakob Bach and Klemens Böhm. “Alternative feature selection with user control”. In: *Int. J. Data Sci. Anal.* (2024). DOI: 10.1007/s41060-024-00527-8
- Constrained subgroup discovery (C4):
  - Jakob Bach. *Using Constraints to Discover Sparse and Alternative Subgroup Descriptions*. arXiv:2406.01411v1 [cs.LG]. 2024. DOI: 10.48550/arXiv.2406.01411
  - Jakob Bach. *Subgroup Discovery with Small and Alternative Feature Sets*. Conditionally accepted at SIGMOD 2025.

Related Work

- Integrating domain knowledge and constraints:
  - Feature selection: Typically only combination of one constraint type (like cost [45, 47], cardinality [27, 54], or group [25, 55]) and feature-selection method; exceptions (wrapper methods with black-box constraints): [23, 42]
  - Subgroup discovery: White-box formulations of different problem definitions [18, 35] and integration of constraints into algorithmic search methods [2, 40]
  - Other fields: E.g., AutoML [43], clustering [15], pattern mining [51], XAI [17]; outside ML: software engineering [21]

- Finding alternative solutions:
  - Feature selection: Approaches that offer less user control over alternatives, e.g., ensemble feature selection [24, 50] or statistically equivalent feature sets [12, 30]
  - Subgroup discovery: Subgroup-set selection [36, 48]; different problem definitions of alternative descriptions, e.g., description-based subgroup selection [33] or equivalent subgroup descriptions of minimal length [11]
  - Other fields: E.g., clustering [8], number partitioning [32], subspace search [19], XAI [41]

Future Work

- Different areas/directions: ML methodology, applied ML, and complexity theory

- ML methodology:
  - Integrating constraints into more methods
  - Soft constraints
  - Feature engineering
- Applied ML:
  - Case studies with qualitative interpretation of results
  - User-friendly systems
- Complexity theory:
  - Approximation complexity
  - Parameterized complexity

(C2) Scientific Hypotheses as Constraints – Approach

- Case study on impact of constraints in a specific use case
  - Scenario [52] from materials science: Predict density of dislocation reactions in a specimen under load
  - Constraints express preferences regarding feature sets and hypotheses from domain
  - Idea: Hypotheses inconsistent to data should lower prediction quality significantly

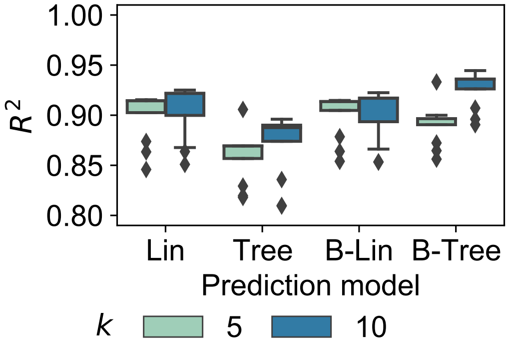
- Experimental design:
  - One dataset with 14,903 data objects, 135 features, and continuous target
  - Linear objective using Pearson correlation as $q(\cdot)$, four prediction models
  - Constraint types: Three domain-independent (preferences) and twelve domain-specific (hypotheses)

Example (Constraint type)

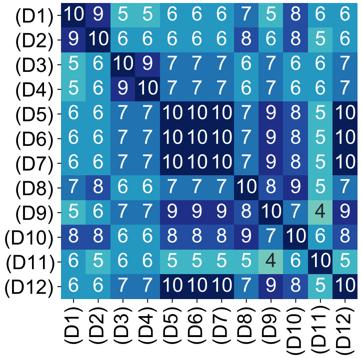
$$\text{Aggregate-or-original}(\{s_1, \dots, s_n\}) = \bigwedge_{p \in P} \left(\left(\bigvee_{a \in A} s_{(p,a)} \right) + \left(\bigvee_{l \in \{1,\dots,12\}} s_{(p,l)} \right) \leq 1 \right)$$

$\leftrightarrow$ “For each physical quantity p, do not select aggregate features a and original features l at the same time.”

(C2) Scientific Hypotheses as Constraints – Results



Distribution of prediction quality over constraint types (which express scientific hypotheses).



Overlap size of feature sets between constraint types (for selecting $k = 10$ features).

References

(C3) Alternative Feature Selection – Experimental Design

- 30 binary-classification datasets (with 106–9822 data objects and 15–168 features) from *PMLB* [44, 49]
- Five feature-set quality measures as objective functions
- Different search configurations for alternatives:
  - Number of alternatives a
  - Dissimilarity threshold τ
  - Search methods (three solver-based, two heuristics)
- Evaluation metrics:
  - Objective value
  - Prediction performance (MCC [39])
  - Runtime
  - Optimization status
- *SCIP* [9] (a MIP solver) via Google OR-Tools [46] as optimizer for solver-based search

(C4) Subgroup Discovery – Formalization: Alternatives

- Concept: Cover similar set of data objects as given subgroup with different set of selected features
  - Repeat sequentially to get $a \in \mathbb{N}$ alternatives for dissimilarity threshold $\tau \in \mathbb{R}_{\geq 0}$

- Chosen optimization objective: Maximize normalized Hamming similarity (= prediction accuracy)

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

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

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

(C4) Subgroup Discovery – Complexity

- Subgroup discovery with a feature-cardinality constraint is $\mathcal{NP}$-complete
- Proof: Reduction from SET COVERING [26]
  - 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., $X_{(m+1)j} = 0$
    - 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
  - Finally, optimizing subgroup quality typically at least as hard as finding perfect subgroup

(C4) Subgroup Discovery – Experimental Design

- 27 binary-classification datasets (with 106–9822 data objects and 20–168 features) from *PMLB* [44, 49]
- Six subgroup-discovery methods:
  - Solver-based (novel): *SMT* (using *Z3* [10, 16] as optimizer)
  - Heuristics (related work): *Beam*, *BI* [37], *PRIM* [20]
  - Baselines (novel): *MORS* (Minimal Optimal Recall Subgroup), *Random*
- Four experimental scenarios: Unconstrained, two constraint types, and solver timeouts
  - Solver timeouts: {1 s, 2 s, 4 s, . . . , 2048 s}
  - Feature-cardinality constraints: $k \in \{1, 2, 3, 4, 5\}$
  - Alternative subgroup descriptions: $k = 3$, $a = 5$, and $\tau_{\text{abs}} \in \{1, 2, 3\}$
- Evaluation metrics:
  - Subgroup quality (nWRAcc [31, 38])
  - Runtime
  - For alternatives: Similarity [14] (Normalized Hamming and Jaccard)

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