

Finding Optimal Solutions for Alternative Feature Selection

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Abstract—Feature-selection methods are popular for obtaining small, interpretable, yet highly accurate prediction models. Existing feature-selection methods typically yield only one feature set, which might not be sufficient in some cases. For example, users might be interested in finding different feature sets with similar prediction quality, offering alternative explanations of the data. In this article, we formalize alternative feature selection as an optimization problem. Next, we propose several general approaches to solve this problem. In particular, we show how to integrate various categories of existing feature-selection methods. Finally, we evaluate these approaches in a study with 30 classification datasets. In our experiments, we are able to determine alternative feature sets with high prediction quality.

Index Terms—feature selection, alternatives, constraints, explainability, interpretability

I. INTRODUCTION

a) Motivation: Feature-selection methods are ubiquitous for various reasons. By reducing dataset dimensionality, they lower the computational and memory requirements of prediction models. Next, models might generalize better if irrelevant and spurious predictors are removed. Finally, prediction models might be smaller and more comprehensive due to feature selection [1], improving interpretability.

Traditional feature-selection methods mostly return only one feature set [2]. These methods optimize a criterion of feature-set quality, e.g., prediction performance. However, besides the optimal feature set, there might be other, differently composed feature sets with similar quality. For the user, these alternative feature sets might be interesting for multiple reasons. First, some originally selected features might be costly to obtain, so the user would prefer cheaper alternatives. Second, some originally selected features might contain sensitive information that should not be used in predictions. Third, the user might be interested in explanations for the prediction. In such a situation, knowing alternatives allows the formulation of multiple hypotheses and broadens the understanding.

b) Problem statement: This article addresses the problem of alternative feature selection, which we define as follows:

Definition 1 (Alternative feature selection (informal)). Given an original set of features, find a sufficiently different set that optimizes feature-set quality at the same time.

We will provide formal definitions later. Depending on how different the alternative feature set should be composed, one

might have to compromise on quality. E.g., if the original feature set already contains most of the highly predictive features, the alternative might have significantly lower quality. We analyze this effect in our article. Also, we consider finding multiple alternatives rather than just one.

Two points are essential for alternative feature selection, which we both address in this article. First, one needs to formalize and quantify what an alternative feature set is. Second, one needs an approach to find alternative feature sets efficiently. Ideally, the approach should be general, i.e., cover a broad range of existing feature-selection methods.

c) Related work: In machine learning, finding alternative solutions has already been addressed extensively in clustering [3]. However, there is a lack of such approaches and corresponding experimental evaluation for feature selection. Only a few feature-selection methods target at obtaining multiple, diverse feature sets [2], [4]. Techniques for ensemble feature selection [5], [6] and statistically equivalent feature subsets [7] produce multiple feature sets but do not focus on optimal alternatives. In the field of explainable AI, counterfactual explanations have massively gained popularity in the last few years [8], [9]. Such explanations involve data objects with similar feature values but a different prediction outcome. In contrast, we target at different feature sets but similar feature-set quality, e.g., prediction performance.

d) Contributions: Our contribution is threefold. First, we formalize alternative feature selection as an optimization problem. In particular, we foster alternatives via constraints on feature sets. Second, we propose heuristic and exact approaches to solve this optimization problem. To that end, we discuss how to integrate different categories of feature-selection methods in the objective function. Our notion of alternative feature sets is general and thus not tailored towards specific feature-selection methods. Third, we evaluate our approaches for alternative feature selection with comprehensive experiments. We use 30 classification dataset from the Penn Machine Learning Benchmarks (PMLB) [10], [11] and four different feature-selection methods. We focus on the question if one can find alternative feature sets with similar feature-set quality as the original ones.

e) Results: Our experiments show that finding alternative feature sets with similar quality is possible indeed. This outcome encourages using alternative feature sets as a tool for

alternative explanations of predictions. As expected, feature-set quality tends to decrease with the number of alternatives. Naturally, the exact decrease depends on the dataset and how feature-set quality is distributed. Further, we note that the quality of alternative feature sets significantly depends on the dissimilarity threshold for being alternative. Thus, this threshold allows the user to exercise control over alternatives and make use-case-specific choices.

We publish our code¹ and our experimental data² online.

f) Outline: Section II explains fundamentals of feature selection. Section III defines the optimization problem of alternative feature selection and discusses approaches to solve it. Section IV reviews related work. Section V describes our experimental design. Section VI presents the experimental results. Section VII concludes.

II. FUNDAMENTALS

In this section, we introduce basic notation and review different methods to measure the quality of feature sets.

A. Notation

Let $X \in \mathbb{R}^{m \times n}$ be a dataset represented as a matrix. Each row is a data object, and each column is a feature. Let $F = \{f_1, \dots, f_n\}$ denote the set of feature names. We assume categorical features have already been made numeric, e.g., via one-hot encoding. Let $X_{\cdot j} \in \mathbb{R}^m$ denote the vector representation of the j -th feature. Further, let $y \in \mathbb{R}^m$ represent the prediction target. The actual domain of the target might also be smaller, e.g., $\{0, 1\}$ for binary classification.

With feature selection, one makes a binary decision $s_j \in \{0, 1\}$ for each feature, i.e., either selects it or not. The vector $s \in \{0, 1\}^n$ combines all these selection decisions. The selected feature set is $F_s = \{f_j \mid s_j = 1\}$. Let the function $Q(s, X, y)$ return the quality of such a feature set. Without loss of generality, we assume this function should be maximized.

B. Measuring Feature (Set) Quality

There are different ways to evaluate feature-set quality $Q(s, X, y)$. Note that we only give a short overview here. See [12], [1] for comprehensive surveys of feature selection. A typical categorization of feature selection is into filter, wrapper, and embedded methods [13].

a) Filter methods: Filter methods evaluate feature sets without training a prediction model. Univariate filters assess each feature independently, while multivariate filters evaluate feature sets. Examples of univariate filters are the Pearson correlation or the mutual information between a feature and the prediction target. Such methods ignore the interaction between features, e.g., redundancies. Multivariate methods, like CFS [14], FCBF [15], and mRMR [16], often combine a measure of feature relevance with a measure of feature redundancy to express feature-set quality.

b) Wrapper methods: Wrapper methods [17] assess feature-set quality by training a prediction model with the feature set and evaluating prediction performance. Wrappers can use an arbitrary black-box optimization strategy to iterate over feature sets, e.g., genetic algorithms.

c) Embedded methods: Embedded methods have feature selection built into the training of prediction models, e.g., decision trees [18] or random forests [19]. Thus, the criterion to evaluate feature-set quality is model-specific. Tree-based models typically use information gain or the Gini index.

d) Post-hoc feature-importance methods: Apart from traditional feature selection, various methods assess feature importance after training a model. Assessing feature importance plays a crucial role in the emerging fields of ML interpretability [20]. Approaches range from local explanation methods, like LIME [21] or SHAP [22], to global importance methods, like permutation importance [19] or SAGE [23].

III. ALTERNATIVE FEATURE SELECTION

In this section, we present the problem and approaches for alternative feature selection. First, we give an overview of the optimization problem. Second, we formalize the notion of alternatives via constraints. Third, we discuss different objective functions corresponding to different feature-set quality measures from Section II-B. In particular, we describe how to solve the resulting optimization problem.

A. Optimization Problem

In alternative feature selection, there are two goals. First, the quality of an alternative feature set should be high. Second, an alternative feature set should differ from one or more existing feature set(s). There are different ways to combine these two goals in an optimization problem:

First, one can consider both goals as objectives, obtaining an unconstrained multi-objective problem. Second, one can treat feature-set quality as objective and enforce alternatives with constraints. Third, one can consider being alternative as objective and constrain feature-set quality, e.g., with a lower bound. Fourth, one can define constraints for both, feature-set quality and being alternative, searching for feasible solutions instead of optimizing. Depending on the use case, any of these four formulations might be appropriate.

Following the informal Definition 1 from the introduction, we stick to the second formulation, i.e., optimizing feature-set quality subject to being alternative. This formulation has the advantage of keeping the original objective function of feature selection. Consequently, one does not need to specify a range or a threshold on feature-set quality. Instead, the user can control how alternative the new feature set should be. This yields the following optimization problem:

$$\begin{aligned} \max_s \quad & Q(s, X, y) \\ \text{subject to:} \quad & F_s \text{ being alternative} \end{aligned} \tag{1}$$

We discuss different constraints for *being alternative* and different objective functions $Q(s, X, y)$ in the following.

¹temporary, anonymized version for review: <https://www.dropbox.com/sh/s1n5vxfugtfurm/AACecUHOZvrEq9EHg6KHXAvgA?dl=0>

²temporary, anonymized version for review: <https://www.dropbox.com/sh/3bmeoihgozmvfg3/AAD9AcRddqRVlu7tps6FxiKIa?dl=0>

B. Constraints – Defining Alternative Feature Sets

In this section, we formalize alternative feature sets. This part of our work is independent of the feature-selection method. First, we discuss the base case where an individual feature set is an alternative to another one. Second, we extend this notion to multiple alternatives, considering sequential as well as simultaneous search procedures.

1) *Single Alternatives*: We consider a feature set to be an alternative to another feature set if it differs sufficiently. Mathematically, we express this with a set-dissimilarity measure [24]. Most of these measures describe how strongly two sets overlap and set this in relation to the size of the sets. In our article, we base dissimilarity on the Dice coefficient, a well-known and straightforward set-similarity measure:

$$d_{Dice}(F_1, F_2) = 1 - \frac{2 \cdot |F_1 \cap F_2|}{|F_1| + |F_2|} \quad (2)$$

We leverage such a set-dissimilarity measure for the following definition:

Definition 2 (Single alternative). A feature set F_2 is an alternative to a feature set F_1 (and vice versa) for a dissimilarity threshold $\tau \in \mathbb{R}_{\geq 0}$ if $d(F_1, F_2) \geq \tau$.

Depending on the preferences of the user, different values of τ might be appropriate. τ controls how alternative the new feature set should be. A feature set that differs strongly might cause a significant drop in feature-set quality. Thus, we leave τ as a parameter. If the set-dissimilarity measure $d(\cdot)$ is normalized to $[0, 1]$, like the Dice dissimilarity, the interpretation of τ is user-friendly: A value of 0 allows the alternative feature set to be identical to the original one. A value of 1 requires the two feature sets to have no overlap.

If the feature sets sizes $|F_1|$ and $|F_2|$ are known, a threshold τ corresponds to a particular maximum number of overlapping features $|F_1 \cap F_2|$. This follows from re-arranging Equation 2 in combination with Definition 2:

$$d_{Dice}(F_1, F_2) \geq \tau \Leftrightarrow |F_1 \cap F_2| \leq \frac{1 - \tau}{2} \cdot (|F_1| + |F_2|) \quad (3)$$

The latter formulation also avoids having the feature-set sizes, and thereby the decision variables for feature selection, in a quotient. We can see that the effect of setting τ on the maximum overlap size $|F_1 \cap F_2|$ is linear. For the Jaccard distance, another popular set-dissimilarity measure, we would obtain a non-linear expression regarding τ .

If we additionally require $|F_1| = |F_2|$, the parameter τ directly controls which fraction of features in one set needs to differ from the other set, and vice versa:

$$\begin{aligned} &\text{If } |F_1| = |F_2| : d_{Dice}(F_1, F_2) \geq \tau \\ &\Leftrightarrow |F_1 \cap F_2| \leq (1 - \tau) \cdot |F_1| = (1 - \tau) \cdot |F_2| \end{aligned} \quad (4)$$

Up to now, we have worked with feature set sizes instead of the binary feature-selection vector s . However, expressing the feature-set sizes in terms of s is straightforward:

$$|F_s| = \sum_{j=1}^n s_j \quad \text{and} \quad |F_{s_1} \cap F_{s_2}| = \sum_{j=1}^n s_{1,j} \cdot s_{2,j} \quad (5)$$

Combining Equation 3 with Equation 5 yields an inequality only involving sums and products of the decision variables and constants. In fact, one can replace the product $s_{1,j} \cdot s_{2,j}$ with linear constraints by introducing an auxiliary variable t_j [25]:

$$\begin{aligned} t_j &\leq s_{1,j} & t_j &\leq s_{2,j} \\ 1 + t_j &\geq s_{1,j} + s_{2,j} & t_j &\in \{0, 1\} \end{aligned} \quad (6)$$

If there is an existing feature set, i.e., we either know s_1 or s_2 , Equation 5 already is linear without Equation 6.

Overall, one can express alternative feature sets according to Definition 2 with 0-1 integer linear constraints. This simple constraint type allows using a broad range of solvers, given a suitable objective function, which we discuss later.

2) *Multiple Alternatives*: If the user desires multiple alternative feature sets rather than just one, we can compute these alternatives either sequentially or simultaneously.

a) *Sequential alternatives*: In the sequential case, we obtain alternatives iteratively, with one alternative feature set per iteration. We constrain the new feature set to be an alternative to all previously found feature sets:

Definition 3 (Sequential alternative). A feature set F_2 is an alternative to a set of feature sets \mathbb{F} (and vice versa) for a dissimilarity threshold $\tau \in \mathbb{R}_{\geq 0}$ if $\forall F_1 \in \mathbb{F} : d(F_1, F_2) \geq \tau$.

This definition duplicates the constraint from the base case and instantiates it for different existing feature sets. One could also use a less strict constraint, e.g., requiring only the average dissimilarity to all existing feature sets to pass the threshold. The objective function remains the same as in the base case, i.e., we only optimize the quality of the new feature set F_2 . Thus, the number of variables in the optimization problem remains constant, independent of the number of alternatives. Further, we do not need to introduce interaction variables as in Equation 6. Each alternative only adds one new constraint to the optimization problem. Thus, we expect the runtime of sequential search to scale well with the number of alternatives. Further runtime gains might be possible if the solver keeps a state between iterations and can warm-start. Regarding feature-set quality, we expect a drop with each alternative, as the solution space becomes narrower over iterations. After each iteration, the user can decide if the feature-set quality is too low or if another alternative should be found.

b) *Simultaneous alternatives*: In the simultaneous case, we directly obtain several alternatives. The user needs to decide on the number of feature sets \mathbb{F} beforehand. We formulate pairwise dissimilarity constraints:

Definition 4 (Simultaneous alternative). A set of feature sets \mathbb{F} contains simultaneous alternatives for a dissimilarity threshold $\tau \in \mathbb{R}_{\geq 0}$ if $\forall F_1 \in \mathbb{F}, F_2 \in \mathbb{F}, F_1 \neq F_2 : d(F_1, F_2) \geq \tau$.

Again, one could resort to less strict constraints, e.g., based on the average dissimilarity between alternatives. In contrast to the sequential case, we need to introduce further decision variables and modify the objective function here, as we optimize multiple feature sets at once. In this paper, we consider the summed quality of all feature sets as the objective.

Runtime-wise, we expect simultaneous search to scale worse with the number of alternatives than sequential search. The number of decision variables increases linearly with the number of alternatives, while the number of constraints grows quadratically. Also, for each feature and each pair of alternatives, we need to introduce an interaction variable as in Equation 6 if we want to obtain a linear problem.

In contrast to the greedy procedure of sequential search, simultaneous search optimizes alternatives globally. Thus, the simultaneous procedure should yield higher average feature-set quality for the same number of alternatives. Also, we expect the qualities of the alternatives to be more evenly distributed, as opposed to the dropping quality over the course of the sequential procedure.

C. Objective Functions – Finding Alternative Feature Sets

In this section, we present concrete approaches for finding alternative feature sets. We discuss how to solve the optimization problem from Section III-A for the different categories of feature-set quality measures from Section II-B. In particular, we categorize solution approaches as white-box optimization, black-box optimization, and embedding alternatives.

1) *White-Box Optimization*: If the feature-set quality function $Q(s, X, y)$ is sufficiently simple, one can tackle alternative feature selection with a white-box solver.

a) *Univariate filter feature selection*: For univariate filter feature selection, the objective function is linear. Thus, the optimization problem of alternative feature selection becomes a 0-1 integer linear problem. In particular, univariate filter methods decompose the quality of a feature set into the quality of the individual features:

$$Q_{uni}(s, X, y) = \sum_{j=1}^n s_j \cdot q(X_{\cdot j}, y) \quad (7)$$

Here, $q(\cdot)$ typically is a bivariate dependency measure, e.g., mutual information [26] or correlation, to quantify the relationship between a feature and the prediction target.

b) *Post-hoc feature importance*: From the technical perspective, one can also insert values of post-hoc feature importance scores for $q(\cdot)$ in Equation 7. For example, one can pre-compute permutation importance [19] or SAGE scores [23] for each feature. However, such post-hoc importance scores often evaluate the usefulness of features under the presence of other features. In consequence, the feature-independence assumption underlying Equation 7 does not hold. However, re-calculating feature importance for each possible feature set makes a white-box approach infeasible. In practice, one can still use Equation 7 with importance scores computed on the full dataset. One only needs to be aware that such an approach might not represent feature interactions faithfully.

c) *Multivariate filter feature selection*: Several multivariate filter methods also enable a simple white-box formulation, though not necessarily a linear one. In the following, we discuss the Fast Correlation-Based Filter (FCBF) [15], which we use in our experiments. CFS [14] and mRMR [16] allow white-box optimization as well [27].

FCBF bases on the notion of predominance: It strives to select features with at least a certain correlation to the prediction target but a lower correlation to all other features. While the original FCBF algorithm uses a heuristic search, we propose a formulation as a constrained optimization problem:

$$\begin{aligned} \max_s \quad & Q_{FCBF}(s, X, y) = \sum_{j=1}^n s_j \cdot q(X_{\cdot j}, y) \\ \text{subject to:} \quad & \forall (j_1, j_2) \in \{1, \dots, n\}^2, j_1 \neq j_2 : \\ & s_{j_1} \cdot s_{j_2} \cdot q(X_{\cdot j_1}, X_{\cdot j_2}) < q(X_{\cdot j_1}, y) \end{aligned} \quad (8)$$

We drop the original FCBF’s threshold parameter on feature-target correlation and maximize the latter instead, as in the univariate filter case. With the constraint in Equation 8, we enforce that if two features are selected, their correlation has to be lower than each feature’s target correlation. Overall, the optimization problem is linear again if one appropriately handles the product term between decision variables.

2) *Black-Box Optimization*: If feature-set quality has no closed-form expression, one can treat it as a black-box function when searching for alternative feature sets. This situation applies to the category of wrapper feature selection. One can optimize such black-box functions using search heuristics, systematically iterating over candidate feature sets.

However, search heuristics often assume an unconstrained search space. For example, they might propose a candidate feature set that is not alternative enough. We see multiple ways to address this challenge: First, one can enumerate and evaluate all feature sets satisfying the constraints, which is inefficient. Second, one can sample valid feature sets, which is not easy if the procedure should sample uniformly [28]. Third, one can formulate a multi-objective problem, so there are no hard constraints on alternatives anymore. Fourth, one can adapt a search heuristic to consider constraints; this is what we describe in the following.

There are several approaches for adapting search heuristics to constraints. One idea is to prevent a search heuristic from producing feature sets that violate the constraints or at least make the latter less likely, e.g., by penalizing the objective function accordingly. Another idea is to ‘repair’ feature sets proposed by the search that are not alternative enough. For example, one can replace a feature set violating the constraints with the most similar feature set satisfying the constraints. Such solver-assisted search approaches are common in the search for software configurations [29], [30], [31].

As a simple wrapper approach for our experiments, we use a greedy hill-climbing strategy, as displayed in Figure 1. Compared to standard hill-climbing [17], our search only evaluates feature sets that satisfy the constraints for alternatives. First, the algorithm uses a solver to find one sufficiently alternative solution. Next, it tries ‘swapping’ a feature, i.e., selecting the feature if it was deselected or deselecting it if it was selected. The algorithm applies the solver again to find a solution s' containing this change and satisfying the other constraints. If such a solution s' exists and its quality $Q(s', X, y)$ improves the current solution, the algorithm continues from the new

Input: Dataset X , Prediction target y ,
Feature-set quality function $Q(\cdot)$,
Constraints for alternatives $Cons$,
Maximum number of iterations max_iters

Output: Feature-selection decision vector s

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1  $s \leftarrow \text{Solve}(Cons)$  // Initial alternative
2  $iters \leftarrow 1$  // Number of solver calls
3 if  $s = \emptyset$  then return  $\emptyset$  // No alternative
4  $j \leftarrow 1$  // Index to be swapped
5 while  $iters < max\_iters$  and  $j \leq |s|$  do
6    $s' \leftarrow \text{Solve}(Cons \cup \{\neg s_j\})$  // Swap feature
7    $iters \leftarrow iters + 1$ 
8   if  $s' \neq \emptyset$  and  $Q(s', X, y) > Q(s, X, y)$  then
9      $s \leftarrow s'$  // Swap if improved
10     $j \leftarrow 1$ 
11  else  $j \leftarrow j + 1$  // Try next feature
12 return  $s$ 

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Fig. 1. Constraint-aware greedy wrapper feature selection.

solution. Else, it attempts to swap the next feature. The algorithm terminates if no swap leads to an improvement or a fixed number of iterations max_iters is reached. Each iteration corresponds to one solver call and, if the solver yields a valid feature set, one training of the prediction model.

3) *Embedding Alternatives*: If feature selection is embedded into training a prediction model, there is no general approach for finding alternative feature sets. Instead, one would need to embed the search for alternatives into training as well. For example, one could prevent decision trees from splitting on a feature if the resulting feature set was too similar to an existing feature set. We leave the formulation of such specific approaches open for future work.

IV. RELATED WORK

In this section, we review literature from areas related to alternative feature selection: alternative clustering, subspace search, feature selection, and counterfactual explanations. To the best of our knowledge, searching for optimal alternative feature sets is novel. However, there is literature on optimal alternatives outside the field of feature selection. Also, there are works on finding multiple, diverse feature sets.

a) *Alternative clustering*: Finding alternative solutions has been addressed extensively in the field of clustering. [3] gives a taxonomy of alternative clustering and describes algorithms from different categories of alternative clustering. Our problem definition in Sections III-A and III-B is, on a high level, inspired by the one in [3]: find one or multiple solutions that maximize quality while minimizing similarity. [3] also distinguishes between singular alternatives and multiple alternatives, found sequentially or simultaneously. Nevertheless, the concrete problem definition for our feature-selection scenario is different.

b) *Subspace search*: Finding multiple feature set plays a role in subspace clustering [32], [33], [34] and subspace search [35], [36], [37]. These approaches strive to improve the results of data-mining algorithms by using subspaces, i.e., feature sets, rather than the full space, i.e., all features. Some subspace approaches explicitly try to remove redundancy between subspaces [32], [35] or foster subspace diversity [36], [37], which bears some resemblance to alternative feature selection. Nevertheless, the scenarios are fundamentally different, e.g., we are in a supervised setting.

c) *Feature selection*: Most feature-selection methods only yield one solution [2], though there are some exceptions. Nevertheless, none of the following approaches explicitly searches for optimal alternatives. [4] adapts a genetic algorithm to ensure diversity of feature sets by penalizing overlap of feature sets. [38] uses multi-objective genetic algorithms to obtain prediction models that use feature sets of different sizes. [39] clusters features based on their values and then forms all combinations of picking one feature from each cluster. [40] presents six strategies to foster diversity in subgroup set discovery, which searches for interesting regions in the data space rather than explicitly selecting features.

d) *Ensemble feature selection*: Ensemble feature selection [5], [6] runs feature selection on different versions, e.g., samples, of the data or uses different feature-selection methods. While fostering diverse feature sets might be a sub-goal, the results of the different feature selectors are combined at the end. Thus, this focus is different from ours. As an example, [41] uses clustering and frequent-itemset mining to reduce a set of feature-selection results, obtained on bootstrap samples of the data, to a smaller, yet diverse set. [42] builds an ensemble prediction model from classifiers trained on different feature sets and uses an evolutionary algorithm that ensures diversity of feature sets. [43] selects features separately for each class and then combines the results.

e) *Statistically equivalent feature sets*: A subfield of feature selection is the search for statistically equivalent feature sets [7], [2]. These approaches use statistical tests to determine which features or feature sets can be used interchangeably to predict a target. While equivalent feature sets are related to our notion of alternative feature sets, there are differences as well. Depending on the configuration of statistical tests, there can be an arbitrary number of equivalent feature sets, without an explicit ordering. Instead, we always provide a fixed number of alternatives. Rather than striving for equivalence between feature sets, we optimize under constraints. Our dissimilarity threshold allows controlling the overlap of feature sets instead of eliminating all feature redundancies. Nevertheless, if one wants to prevent the selection of certain redundant features or feature sets reliably, one can achieve this with additional constraints in our optimization problem as well.

f) *Constrained feature selection*: There is work on considering various kinds of constraints in feature selection, e.g., for costs [44], feature group [45], or domain-knowledge [46]. These approaches are orthogonal to our work, as such constraints can be added to our optimization problem as well.

g) *Counterfactual explanations*: Alternative feature selection shares some similarities with the concept of counterfactual explanations for predictions [8], [9]. Counterfactual explanations also provide alternative solutions and might be formulated as optimization problem [47], [48]. In particular, [49] presents an approach to find diverse counterfactual explanations. However, there are crucial differences between counterfactuals and alternative feature sets: Counterfactual explanations target at predictions on single data objects rather than the global predictive quality of features. Also, counterfactuals want to alter the prediction outcome by changing feature values little, while alternative feature sets should keep the prediction quality while changing the feature set significantly.

V. EXPERIMENTAL DESIGN

In this section, we describe our experimental design. First, we give a brief overview of its goal and components. Next, we elaborate on different components of the design in detail.

A. Overview

We conduct experiments with 30 datasets for binary classification. In our evaluation, we mainly focus on the trade-off between feature-set quality and obtaining alternative feature sets. We compare four feature-selection methods, representing different notions of feature-set quality. Also, we train prediction models with the resulting feature sets and analyze prediction performance. To find multiple alternative feature sets, we consider a simultaneous as well as a sequential approach. We systematically vary the number of alternatives and the dissimilarity threshold for being alternative.

B. Methods

1) *Feature Selection (Objective Functions)*: To have a diverse set of feature-selection methods, we consider the different categories from Section II-B. We choose four well-known feature-selection methods that are either parameter-free or easy to parameterize. See Section III-C for details on the objective function of each method. One method (*Greedy Wrapper*) requires black-box optimization, while the other three methods have white-box objectives. As explained in Section III-C3, we do not include an embedded method.

For each feature-selection method, we set the number of selected features to $k \in \{5, 10\}$. These values yield small feature sets, fostering interpretability. We enforce the desired k with a simple constraint in our optimization problems.

a) *MI*: For univariate filtering, we use Equation 7 with mutual information [26] as dependency measure $q(\cdot)$. To improve comparability between datasets and values of k , we normalize the qualities such that selecting all features yields a quality of 1 and selecting no feature yields a quality of 0.

b) *FCBF*: As a multivariate filter method, we use our constrained formulation of FCBF [15] according to Equation 8. As bivariate quality measure within FCBF, we rely on mutual information again, normalized to sum up to 1.

c) *Greedy Wrapper*: As a wrapper method, we employ a greedy hill-climbing strategy according to Algorithm 1. We set *max_iters* to 1000. To evaluate feature-set quality within the wrapper, we choose a decision tree as the prediction model and Matthews correlation coefficient (MCC) [50] as the performance metric. Also, we apply a stratified 80:20 holdout split to test generalization performance. Thus, $Q(s, X, y)$ corresponds to the MCC on the 20% validation part of the data.

d) *Model Gain*: As a post-hoc importance measure, we take model-based feature importance provided by *scikit-learn*. Again, we use a decision tree as the model. There, importance expresses a feature's contribution towards optimizing the split criterion of the tree, for which we choose information gain, i.e., mutual information. We plug the importances into Equation 7, i.e., treat the importances like univariate filter scores. Note that the interpretation is different, though. Here, the scores originate from trees trained with all features rather than assessing features in isolation. The model-based importances are normalized to sum up to 1 by default.

2) *Alternatives (Constraints)*: We employ *sequential* as well as *simultaneous* search for alternatives, using the corresponding definitions from Section III-B2. We evaluate 1 to 10 alternatives for sequential search, while we examine 1 to 5 alternatives for simultaneous search. This difference stems from the increased runtime for simultaneous search. For the dissimilarity threshold τ , we analyze all possible sizes of the overlap, or rather the difference, between feature sets. Thus, for $k = 5$, we consider values of τ from 0.2 to 1 with a step size of 0.2, corresponding to an overlap of four to zero features. For $k = 10$ we consider values of τ from 0.1 to 1 with a step size of 0.1. Naturally, we exclude $\tau = 0$, which would allow returning multiple identical feature sets.

Solver runtime may vary considerably even for optimization problems of the same size, so we set a timeout of 60 s on each solver run. If the solver finishes before the timeout, it either finds an optimal solution or proves no solution exists. These two outcomes apply to 94% of the feature sets in our evaluation. In the remaining cases, the solver either found a feasible but potentially suboptimal solution or found no solution though one might exist.

3) *Prediction*: As prediction models, we use decision trees [18] as well as random forests with 100 trees [19]. Both types of models allow learning of complex, non-linear dependencies from the data. We mainly use the default hyperparameters of the models, apart from choosing information gain as the split criterion, to be consistent with filter feature selection, and setting a random seed for reproducibility.

Note that tree models carry out feature selection themselves, i.e., they are embedded approaches. Thus, they need not use all features that we provide to them. However, this is no problem for our study. We are interested in which performance the models achieve if they are limited to small alternative feature sets, not how they use each feature from an alternative.

C. Evaluation Metrics

We use two kinds of metrics for feature-set quality. First, we evaluate the objective functions of the feature-selection methods, which guided the search for feature sets. Second, we train prediction models with the found feature sets. We report prediction performance in terms of the Matthews correlation coefficient (MCC), which is insensitive to class imbalance. This coefficient reaches its maximum of 1 for perfect predictions and is 0 for random guessing.

To analyze generalization, we conduct stratified 10-fold cross-validation. Not only model training but also the search for alternative feature sets is limited to the training data.

D. Datasets

We evaluate alternative feature selection on a variety of datasets from the Penn Machine Learning Benchmarks (PMLB) [10], [11]. To focus the evaluation on one machine-learning task, we only consider binary-classification datasets. However, alternative feature selection is possible for regression and multi-class problems as well. We filter out datasets containing less than 100 instances. Also, we filter out datasets with less than 15 features to leave some room for alternatives. Next, we remove one dataset with 1000 features, which would dominate the overall runtime of the experiments. Finally, we manually remove datasets that seem to be duplicated or modified versions of other datasets from the benchmark.

In consequence, we obtain 30 datasets. The number of data objects varies from 106 to 9822, and the number of features ranges from 15 to 168. The datasets contain no missing values. Categorical features have an ordinal encoding by default.

E. Implementation

We implement our experiments in Python. For machine learning, we use the package *scikit-learn* [51]. To express and solve the constraint optimization problems, we use the solver *CBC* via the package *OR-Tools* [52].

VI. EVALUATION

In this section, we evaluate our experiments. In particular, we discuss results for the different dimensions of our experimental design: datasets, prediction models, feature-selection methods, and approaches to search for alternatives.

A. Datasets

Naturally, feature-set quality depends on the dataset. For example, the distribution of feature-set quality might be relatively uniform or relatively skewed. Datasets with more features n generally allow for more alternative feature sets. At the same time, the (normalized) feature quality $q(X_{:j}, y)$ can be spread over more features than for smaller datasets, making it harder to compose a high-quality feature set.

Indeed, our experiments show a broad variation of feature-set quality over datasets. Further, we do not observe a clear relationship between dimensionality n and feature-set quality.

Q_{train}	1	0.67	0.21	0.38	0.21	0.38
Q_{test}	0.67	1	0.15	0.44	0.15	0.45
MCC_{train}^{tree}	0.21	0.15	1	0.46	0.99	0.51
MCC_{test}^{tree}	0.38	0.44	0.46	1	0.46	0.94
MCC_{train}^{forest}	0.21	0.15	0.99	0.46	1	0.51
MCC_{test}^{forest}	0.38	0.45	0.51	0.94	0.51	1
	Q_{train}	Q_{test}	MCC_{train}^{tree}	MCC_{test}^{tree}	MCC_{train}^{forest}	MCC_{test}^{forest}

Fig. 2. Correlation between evaluation metrics over all experimental settings.

B. Prediction Models

As one can expect, the average prediction performance of random forests is higher than for decision trees. Also, overfitting occurs for both model types, i.e., there is a gap between training-set and test-set prediction performance. This observation is expected as we do not regularize or prune the trees. However, this will not invalidate our analysis of how prediction performance develops over alternatives, where we normalize feature-set quality. The optimization objective Q also shows overfitting for all feature-selection methods, though to a lesser extent than prediction performance.

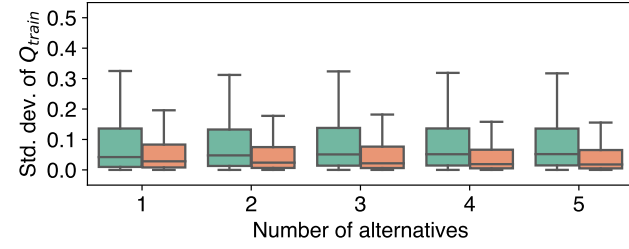
Figure 2 shows the Spearman correlation between different evaluation metrics. As the performance of decision trees and random forests is highly correlated, we focus on decision trees in the following, which always consider all features rather than randomly subsampling them.

Figure 2 also shows that the correlation between training-set quality and test-set quality is moderate, but not high, for the optimization objective Q as well as prediction performance in terms of MCC. This observation might be an effect of overfitting. Further, the correlation between Q and MCC is only weak to moderate. This means that the quality criterion of feature selection is only partially indicative of prediction performance. In particular, only one of our four feature-selection methods uses prediction performance to assess feature sets.

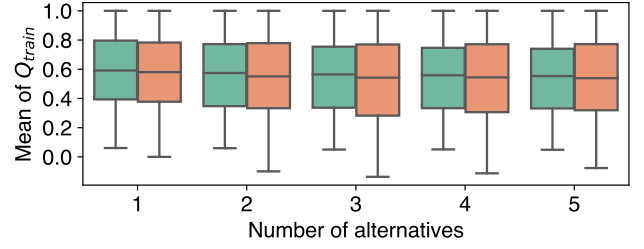
C. Feature-Selection Methods

As the different feature-selection methods have different objective functions, it does not make sense to compare objective values between them. For the optimization status, we note that 89% of feature sets for *FCBF* could not be determined, as the solver timed out or the optimization problem was infeasible. For *MI*, this figure only is 19%. In particular, the additional constraints in our formulation of *FCBF* (c.f. Equation 8) seemingly made it hard to find valid feature sets.

Regarding test-set prediction performance, *Model Gain* is best on average. The median test-set MCC for decision trees is 0.57 for *Model Gain*, 0.54 for *MI*, and 0.51 for *Greedy Wrapper*. It is not surprising that model-based importance

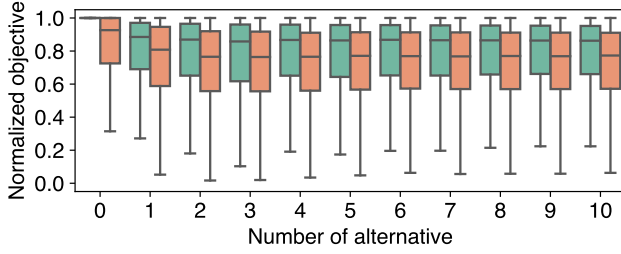


Search sequential simultaneous
(a) Standard deviation of objective.

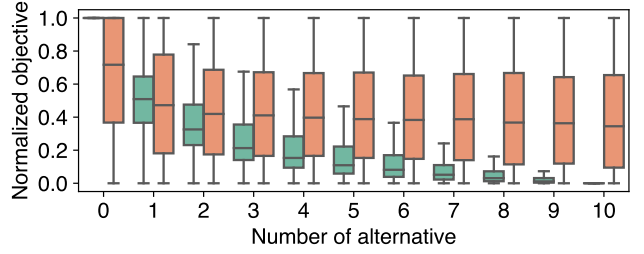


Search sequential simultaneous
(b) Mean objective.

Fig. 3. Training-set objective value Q in experimental runs of sequential or simultaneous search. Outliers removed for readability reasons.



Split train test
(a) Max-normalization.



Split train test
(b) Min-max-normalization.

Fig. 4. Objective value Q , normalized per experimental setting, in sequential search, using MI as feature selector. Outliers removed for readability reasons.

yields better feature sets than univariate, model-free feature scoring with MI . The relatively bad performance of *Greedy Wrapper* might result from its heuristic nature: The wrapper search can only evaluate a fraction of all feasible feature sets and might get stuck in local optima, while the remaining feature-selection methods optimize globally.

The feature-set size k shows expected effects: Larger feature sets, i.e., $k = 10$, yield higher feature-set quality than smaller feature sets, i.e., $k = 5$. However, doubling the number of features does not double prediction performance. Over all experimental settings, the median test-set MCC of decision trees is 0.50 for $k = 5$ and 0.60 for $k = 10$. This shows that small feature sets can already achieve relatively high prediction performance. For the optimization objective Q , the increase from $k = 5$ to $k = 10$ is less than proportional with k as well.

D. Searching Alternatives

1) *Search Method*: As expected, the training-set objective value Q of feature sets within a particular search run varies more for sequential than for simultaneous search. Figure 3a visualizes this observation. Also, the variance slightly increases with the number of alternatives for sequential search but decreases for simultaneous search. I.e., simultaneous search finds more homogeneous feature sets, particularly if many alternatives are desired. However, on the test set, the variance of Q also increases with the number of alternatives for simultaneous search. This effect might be a result of overfitting. Regarding test-set prediction performance, simultaneous search does not even show lower variance than sequential search anymore.

Surprisingly, the average feature-set quality of simultaneous search is not higher than for sequential search, neither regarding objective value Q nor prediction performance. Figure 3b shows this behavior for the mean training-set objective of search runs. Depending on the search setting, either of the two searches might yield better results. An explanation for this phenomenon is that search results might be sub-optimal. Exact optimization can time out, and *Greedy Wrapper* uses a heuristic search per se. As simultaneous search is harder than sequential search, it is affected more by timeouts. In particular, 10% of the feature sets from simultaneous search were feasible but potentially sub-optimal, but no feature sets for sequential search. The former figure strongly depends on the number of alternatives: For up to three alternatives in simultaneous search, less than 1% of feature sets are potentially sub-optimal, but 4% of the feature sets are for four alternatives and 32% of the feature sets for five alternatives. Based on these results, we focus on the sequential search in the following.

2) *Number of Alternatives*: For sequential search, the training-set objective value Q naturally decreases with the number of alternatives, at least for the feature-selection criteria optimized exactly. Figure 4 illustrates this for MI -based feature selection. The other feature-selection methods, including the heuristic *Greedy Wrapper*, exhibit similar effects. As feature-set quality varies between datasets and the number of features k , we apply normalization: In Figure 4a, we have max-normalized the objective value for each search of alternatives, i.e., the highest objective value is scaled to 1. This figure shows that there are multiple alternatives of similar quality, as the

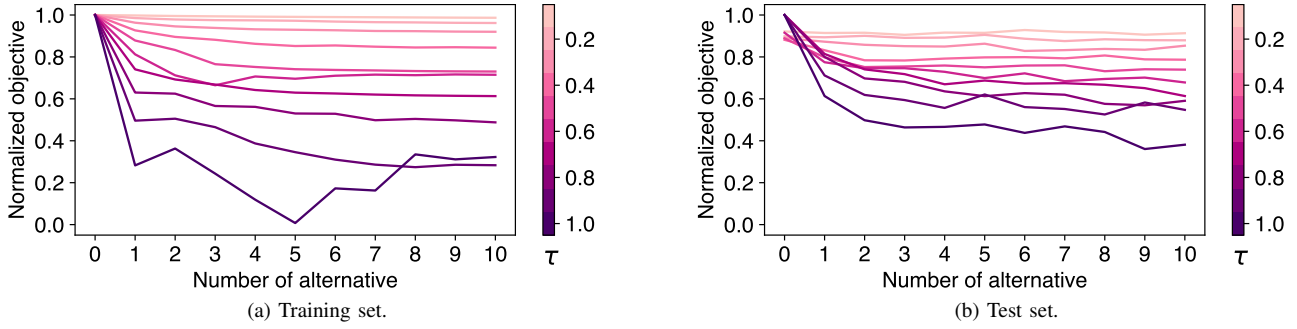


Fig. 5. Median objective value Q , max-normalized per experimental setting, in sequential search, using *MI* as feature selector and $k = 10$.

median feature-set quality remains relatively stable over the number of alternatives and is close to the maximum. Figure 4b uses min-max normalization, i.e., the worst of the alternatives gets 0 as objective. This figure highlights that the training-set objective value decreases most from the original feature set to the first alternative but less beyond.

Additionally, Figure 4 shows that the test-set objective value also drops most to the first alternative. However, the decrease in objective value over the alternatives is less visible than on the training set. In particular, alternatives can even have a higher test-set objective value than the original feature set due to overfitting. Similar findings hold for test-set prediction performance. Thus, the alternative feature sets fulfill their purpose of being different solutions with similar quality.

Be aware that these observations refer to the quality of the found feature sets. However, the more alternatives are desired, the more likely an infeasible optimization problem is. For example, the *MI* feature selector in sequential search always finds an original feature set. However, the problem is infeasible in 2% of the cases for the first alternative, 14% for the second alternative, 24% for the fifth alternative, and 30% for the tenth alternative. This outcome also depends on the dissimilarity threshold τ , which we analyze next.

3) *Dissimilarity Threshold*: As Figure 5 shows for *MI* as feature selector, the decrease of the objective value Q over the number of alternatives can strongly depend on the dissimilarity threshold τ . For a low dissimilarity threshold, e.g., $\tau = 0.1$, the objective value barely drops over the number of alternatives. In contrast, the objective decrease significantly for a high dissimilarity threshold, e.g., $\tau = 1$. This phenomenon also holds for test-set objective and test-set prediction performance, though the decrease with τ is less prominent. Also, the number of infeasible optimization problems, i.e., lack of valid alternative feature sets, increases with τ .

While the prior observations were made for *MI* as the feature selector, they do not hold universally. The results for *Model Gain* strongly depend on τ as well, but the picture for *FCBF* and *Greedy Wrapper* is less clear. For *Greedy Wrapper*, this can be explained by its heuristic search. For *FCBF*, the fraction of infeasible solutions is much higher than for *MI* in general, so adding further constraints has less impact.

VII. CONCLUSIONS AND FUTURE WORK

A. Conclusions

Obtaining interpretable solutions is a highly active area of research in machine learning. One way to foster interpretability is by selecting a small set of features for predictions. Traditional feature-selection methods yield *one* feature set with high quality. However, users might be interested in obtaining multiple, sufficiently different feature sets that, at the same time, have high quality. Such alternative feature sets might provide alternative explanations for predictions.

In this paper, we defined alternative feature selection as an optimization problem. We formalized alternatives via constraints, independent from the feature-selection method. Further, we presented approaches to solve the optimization problem for different categories of feature selectors. Finally, we ran an evaluation with 30 classification datasets and four feature-selection methods. We varied a threshold for how strongly alternatives should differ from existing solutions.

In our experiments, we found that one can obtain alternative feature sets with high feature-set quality. This worked with simultaneous search as well as sequential search for alternatives. The latter procedure was significantly faster and allows stopping the search once one does not want any more alternatives. As expected, the quality of alternatives drops the more alternatives one desires, and the more alternatives should differ. The ultimate decision on which trade-off between feature-set quality and alternatives is acceptable lies with the user. Thus, we recommend evaluating different dissimilarity thresholds for alternatives to find a suitable value.

B. Future Work

While our work introduced alternative feature selection, one might vary several points of our approach. For example, one can integrate other feature-selection methods, particularly embedded methods. Further, one can vary the notion of alternatives, e.g., the set-dissimilarity measure, definition for multiple alternatives, or soft constraints instead of hard constraints. Finally, while our evaluation was domain-independent, the benefit of alternative feature sets for explainable predictions should be analyzed in domain-specific case studies.

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