Feature Selection Methods for Cost-Constrained Classification in Random Forests

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Received: date / Accepted: date

Abstract Cost-sensitive feature selection describes a feature selection problem, where features raise individual costs for inclusion in a model. These costs allow to incorporate disfavored aspects of features, e.g. failure rates of as measuring device, or patient harm, in the model selection process. Random Forests define a particularly challenging problem for feature selection, as features are generally entangled in an ensemble of multiple trees, which makes a post hoc removal of features infeasible. Feature selection methods therefore often either focus on simple pre-filtering methods, or require many Random Forest evaluations along their optimization path, which drastically increases the computational complexity. To solve both issues, we propose Shallow Tree Selection, a novel fast and multivariate feature selection method that selects features from small tree structures. Additionally, we also adapt three standard feature selection algorithms for cost-sensitive learning by introducing a hyperparameter-controlled benefit-cost ratio criterion (BCR) for each method. In an extensive simulation study, we assess this criterion, and compare the proposed methods to multiple performance-based baseline alternatives on four artificial data settings and seven real-world data settings. We show that all methods using a hyperparameterized BCR criterion outperform the baseline alternatives. In a direct comparison between the proposed methods, each method indicates strengths in certain settings, but no one-fits-all solution exists. On a global average, we conclude that a practical analysis should never rely on a single method only, but always compare different approaches to obtain the best results.

Keywords random forest · feature costs · benefit-cost ratio · feature selection · cost-sensitive learning

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1 Background

Cost-constrained feature selection — often also named cost-sensitive learning — describes a statistical modeling problem, where individual costs are assigned to candidate features. These costs may represent financial aspects, but can also be seen as a more general construct referring for example to patient harm during the sample taking process, the failure rate of a measuring device, or a time span to raise a feature. In addition to optimizing predictive performance of the resulting model, cost-constrained feature selection also aims to control the total costs. One way to regulate the costs is to develop flexible approaches harmonizing costs of misclassification and costs of features. Examples of these approaches can be found in Tan (1993), Bolón-Canedo et al. (2014), or Zhou et al. (2016). In this paper we follow a different idea. As flexible approaches require expert knowledge to decide upon the final trade-off, another concept is to simply define a fixed feature cost budget and let the feature selection algorithm find the best possible solution within that constraint region. Research on cost-constrained feature selection with a fixed budget limit can for example be found in Min and Xu (2016), who introduce a novel semi-greedy feature selection approach, Li et al. (2014, 2015), who develop a randomized feature selection strategy focusing on computational efficiency, or Jagdhuber et al. (2020), who introduce cost-adaptations for conventional feature selection methods like genetic algorithms or greedy forward selection for Logistic Regression models. We extend this research by focusing specifically on methods tailored to Random Forest classification and introduce a completely new feature selection idea. Additionally, we also develop cost-sensitive adaptations for existing popular methods in this context.

Random Forests [Breimann, 2001] are an ensemble method of decision trees, which are constructed in a specific way that increases diversity among them. This includes growing each tree on a bootstrap sample of the training data and limiting the set of features for each internal split randomly. Large-scale comparisons by Fernández-Delgado et al. (2014) or Niculescu-Mizil and Caruana (2005) rate Random Forests as state-of-the-art with respect to predictive performance. In the context of cost-sensitive feature selection, these models define a particular challenge, as the actual contribution of individual features is not obvious. This makes the category of wrapper methods for feature selection (Guyon and Elisseeff, 2003) impractical and thus researchers often rely on univariate filter methods. These can be simple approaches like filtering by the individual area under the receiver operating characteristics curve (AUC) (Bommert et al., 2020), but can also be more complex measures to classify the relevance of a feature like for example the permutation feature importance (Breimann, 2001). However, as univariate filter approaches only evaluate features one by one, relevant multivariate aspects might be lost when reducing the dimension of the feature space. On the contrary, more sophisticated methods like greedy sequential forward selection, genetic algorithms (Holland, 1973) or exhaustive approaches, which all incorporate multivariate aspects to their search strategy, generally become computationally prohibitive with increasing data dimensionality.

To solve these problems in a cost-constrained setup, we introduce four feature selection heuristics. The first is a novel algorithm named Shallow Tree Selection (STS). As the name suggests, instead of selecting features directly, STS aims to select tree structures of one or more features. The basis for this selection is provided by specially fitted Random Forests. Each tree represents a (small) multivariate combination of features, which are considered as a connected entity. Unlike in feature importance filters, this property ensures that dependent feature combinations will never be separated during the selection process. From a computational performance standpoint, a big advantage of STS is that it does not need to repeatedly train new Random Forests models to evaluate candidate sets. Instead, all necessary performance components can be computed from the base Random Forest and its out-of-bag samples. In this paper we describe all components of this new method and discuss technical decisions leading to the final implementation. Besides STS, we furthermore propose adaptations of three common feature selection techniques (AUC Filtering, Permutation Feature Importance filtering and Greedy Forward Selection) for cost-sensitive learning by introducing a specialized trade-off metric. This metric weights predictive performance against feature costs to define a harmonized trade-off. It was first described in the $\lambda$-weighted heuristic algorithm by Min et al. (2011) and was further assessed in Min et al. (2014).

To analyze the described methods, we designed an extensive simulation study following the fundamental concepts of Morris et al. (2019). Our main aims are to evaluate strengths and weaknesses of each method, to assess relevant aspects of the trade-off metric, and to give practical recommendations for addressing a cost-sensitive learning problem. We apply all methods on four artificial and six real-world data sets with five pre-defined budget limits each. Results of all proposed methods are evaluated with respect to the mean misclassification error. All conclusions that are drawn from comparisons
of these performance measures are furthermore based on the respective Monte-Carlo errors to account for the uncertainty introduced by the simulation setup.

Section 2 starts by introducing the proposed feature selection heuristics. Special focus is given to our novel STS method. All main concepts and design decisions leading to the final implementation of STS are thoroughly discussed in Subsection 2.1. In the remaining three subsections new cost-sensitive adaptations of AUC Filtering, Permutation Feature Importance Filtering, and Greedy Forward Selection are introduced. Section 3 outlines our simulation study according to the ADEMP scheme of Morris et al. (2019). For a comprehensive overview of all performed analyses, we describe each element of ADEMP in a separate subsection. The results of the simulation study are then presented in Section 4 and discussed in Section 5. In Section 6 we summarize all findings and provide ideas for further research on this topic.

2 Methods

2.1 Shallow Tree Selection (STS)

This section introduces the general idea of STS and thoroughly discusses all concepts that lead to the final method definition. While this approach includes many codependent elements, the general process can be crudely structured into three main steps, which will be discussed in more detail in the following subsections:

1. Generate an ensemble of trees from an adapted Random Forest approach using all candidate features (Subsection 2.1.1).
2. In a greedy forward selection manner, iteratively select the best tree according to a custom trade-off criterion and add it to the result set. Stop the iterative procedure when the available feature cost budget is depleted (Subsection 2.1.2).
3. Re-fit a Random Forest with the implicitly selected feature set of the last ensemble (Subsection 2.1.3).

Section 2.1.4 finally provides a summarizing overview of the final method implementation.

2.1.1 Generating the Base Ensemble

An optimal ensemble of trees contains a diverse set of trees from different combinations of relevant features. The general approach of Random Forests is well-suited here as it creates an ensemble of heterogeneous trees by bootstrapping the data and limiting the feature candidates allowed for each split in the tree growing process. In the context of a feature cost budget, however, the total costs of individual trees play an important role as well. While Random Forests decorrelate the trees in the ensemble, they do not limit the number of features or the total feature costs of a single tree. When budgets are small, or many non-redundant features are relevant, then oftentimes individual trees already exceed the given feature budget. To address this problem, trees with limited costs need to be constructed. However, the implementation of an adapted tree growing algorithm that holds a fixed budget is not trivial, and would for instance need an additional set of rules for the splitting order, when only a fixed set of splits fit the budget. A simple and ready-to-use surrogate solution is to instead define a maximum depth $d_{\text{max}}$ for each tree. Limiting the tree depth corresponds to defining an upper bound of distinct features per tree. While this does not allow the definition of an exact cost budget, it is a practical strategy to scale down the average tree costs. The general formula for the maximum number of features $p$ that a tree with depth $d_{\text{max}}$ can include is $p = 2^{d_{\text{max}}} - 1$.

$d_{\text{max}}$ can be seen as a hyperparameter to regulate the trade-off of complexity and cost. Deep trees are typically more expensive, but also have the ability to describe complex multivariate relations. Very shallow trees often come at little cost and therefore allow greater flexibility in the greedy tree selection steps later. Yet, they only describe small structures, which typically do not perform well on their own. An approach to generally solve the problem of choosing $d_{\text{max}}$ is to combine multiple base forests with $d_{\text{max}} = 1, 2, \ldots, d$. The upper bound $d$ can then for example be set to the maximum value for sensible combinations within the budget limit. By including trees of all depths up to a certain level, it is now for the greedy forward tree selection to decide if the additional costs of a deeper tree is worth its added predictive value. Note that trees with $d_{\text{max}} = 1$ define a special case, where only a single tree per feature is fitted instead of a full Random Forest.
2.1.2 Greedy Forward Tree Selection

After growing an adequate base ensemble of candidate trees \(T = \{T_1, T_2, \ldots, T_{n_{\text{max}}}\}\), an empty result ensemble \(R = \emptyset\) with total cost \(c_R = 0\) is set up. The goal of the subsequent greedy forward selection is to iteratively identify the most suited tree from the base ensemble \(T\) and add it to the result ensemble \(R\). The term most suited is defined by a trade-off criterion that is introduced in the following paragraph.

**Benefit-Cost Ratio Selection Criterion.** In cost-constrained feature selection problems there are two relevant aspects that define the quality of an ensemble. The first aspect is predictive performance. In the context of Random Forests, predictive performance of a single tree can conveniently be evaluated by computing the mean misclassification error (MMCE) on the out-of-bag (OOB) samples of the tree. However, to compute the combined MMCE of an ensemble of trees, it is important not to simply average the individual MMCEs of all trees. This becomes more clear if we for example assume three trees, which classify the same single observation and two of them make a correct prediction, while one misclassifies it. Here, the average of the individual MMCEs is \(\frac{1}{3}\), yet the ensemble itself makes a correct classification and thus has an actual error of 0. To correctly estimate the MMCE, each tree needs to cast a vote for its out-of-bag samples and a majority vote decides in the end on the final classification of each sample. As a practical decision here, we assume samples without a vote to be falsely classified. While this generally results in a too conservative MMCE estimate, it encourages the algorithm to pick trees from different OOB samples to reduce the overall error. The second aspect that defines the quality of a tree ensemble is its total feature cost. This value simply computes as the sum of all costs of included features. In accordance to the generally used definition of cost-sensitive learning, we assume that feature costs are only assigned once per feature and an already ‘paid’ feature can thus be reused without additional costs.

To address both aspects in the greedy forward selection, a trade-off criterion is introduced. The benefit-cost ratio for STS divides the decrease in MMCE of the ensemble \(R\) when adding a tree \(T_i\) by the additional cost that \(T_i\) generates. This allows a combined criterion even though both measures live on different scales. To guide the relative importance of each of these aspects, a hyperparameter \(\xi\) is introduced. The resulting measure is given by

\[
\text{BCR}_{\text{STS}}(T_i, R, \xi) = \frac{\text{MMCE}_{\text{OOB}}((R \cup T_i)) - \text{MMCE}_{\text{OOB}}((R))}{(c_{(R \cup T_i)} - c_{(R)})^{\xi}}.
\]  

(1)

with MMCE(\(\emptyset\)) = 0.5 and \(c_0 = 0\). The BCR can be used to evaluate the impact of adding different candidate trees to an ensemble. The optimal value of this measure is its minimum.

**Selecting the Hyperparameter \(\xi\)** The hyperparameter \(\xi\) allows to control the trade-off between cost and performance. Our main strategy to select \(\xi\) is hyperparameter tuning. In order to tune \(\xi\), a search space, a resampling strategy and a tuning method need to be specified (Bischl et al., 2016). The search space for \(\xi\) is an interval in which the optimal value is expected to lie. As cost is an aspect we aim to penalize, the lower limit of this interval can be chosen as 0. The upper limit however is technically unbounded and needs to be estimated for the problem at hand. The resampling strategy defines the data approach that is used to evaluate the different candidate values. Cross-validation or using a hold-out portion of the data represent typical choices. In the context of Random Forests, a practical strategy is to use the OOB samples as an independent data portion. Finally, the tuning method refers to the algorithm that iteratively proposes new candidates for \(\xi\). A grid search is a simple and practical strategy for this matter. It defines a fixed (equidistant) grid of values within the search space. This makes it robust against local optima. Overall, the hyperparameter tuning strategy described here is comparable to the Competition Strategy, which was proposed in a different context by Min et al. (2013). A faster but more complex alternative is model based optimization (aka Bayesian optimization) (Jones et al., 1998), which is implemented for example in the R package mlrMBO (Bischl et al., 2017). This method is particularly suited for expensive black-box functions and provides a reasonable alternative to optimize \(\xi\) in the STS method.

Besides hyperparameter tuning, we also evaluate alternatives that avoid the optimization of the hyperparameter. These can be formulated as edge cases in terms of \(\xi\). The first such edge case is given by \(\xi = 0\) and is named Cost-Agnostic in the following. With this choice of \(\xi\), the BCR of Equation 1 is reduced to the decrease in MMCE. Hence, individual selection
steps focus on MMCE only, and costs are just considered as a constraint regarding the overall budget limit. A second edge case is $\xi = 1$. This choice can be interpreted as using a simplified BCR without a hyperparameter, like for example found in Paclík et al. (2002), or Leskovec et al. (2007). Compared to the cost agnostic approach, the main appeal of the simple BCR strategy is that it incorporates costs in the selection process, while still avoiding an optimization of $\xi$.

**Candidate Trees without Costs** A final aspect to consider when using a greedy forward selection approach with the BCR criterion of Equation (1) is that trees can become cost-free. That means that at some point, there are candidate trees that only consist of features already present in $R$. Then the denominator of the BCR criterion becomes 0. To avoid this, a decision on how to handle possible cost-free trees needs to be made at the end of each iteration. One option is to add all such trees automatically to the result ensemble. The downside of this approach is that adding a possibly large number of trees at one iteration decreases the impact of all following iterations. For example, the predictions of every single candidate tree to consider in the second iteration may already be outvoted by hundreds of votes from identically structured trees that were added in the first iteration. A further aspect is, that just because a single tree structure is identified to be useful, it does not mean that all existing combinations of those features are.

The alternative option is to remove all cost-free trees from the candidate pool at the end of each iteration. The downside of this approach is that only one structure of each feature combination can be added to the result ensemble. However, as this aspect only has minor effects on the final result and decreasing the pool of candidates furthermore decreases the computational complexity of the algorithm, the latter option was chosen for the STS method.

2.1.3 Feature Selection Result

We continue to add trees from the base ensemble $T$ to the result ensemble $R$, until either $T$ does not contain any further candidate trees, or none of these trees fits the remaining feature cost budget. A specific design aspect of STS is that the algorithm does not aim to build up a highly predictive result ensemble that may then be used as a model. Instead, it only aims to identify well-matching sets of features. Using the ensemble itself as a prediction model would have multiple disadvantages. First, the trees used for STS have limited depth and thus typically cannot compete with their fully grown counterparts. Second, the final ensemble often contains relatively few trees, even if all cost-free trees would be added in the end. As predictive performance of Random Forests increases with the number of trees, the forests constructed in Subsection 2.1.2 generally show relatively poor performance. Therefore, an essential aspect of STS is that it does not focus on the explicit result ensemble itself, but only considers the implicitly selected set of features contained in the trees of the ensemble.

To create the final prediction model, a new Random Forest is fitted from the implicit feature set of the result ensemble. Note that no early stopping of the greedy forward selection is applied. Therefore, the final feature set may still contain a large number of noise features, especially in situations with high budget limits. However, for Random Forests, which usually just ignore noise features, this does not pose a problem.

2.1.4 Summary

This section summarizes all previously introduced design elements and presents a general method overview. A simple working example is given in Figure 1 to illustrate the main principles of STS. The caption of this figure gives a thorough description of each step and refers to relevant subsections for further information.

2.2 Feature Filtering by AUC

To broaden the field of cost-sensitive feature selection methods in Random Forests, we also introduce budget-constraint adaptations for commonly used standard approaches in this context. Because of the computational complexity of this setup, filter methods based for example on Decision Stumps, the Gini-index, or the univariate Area Under the receiver operating characteristic Curve (AUC) (Bommert et al., 2020) are typical choices for feature selection. These methods individually
evaluates the univariate ability of each single feature to separate the response classes. For this paper, we introduce a cost-sensitive adaptation of the AUC filter method. The AUC is a popular trade-off measure, which incorporates both sensitivity and specificity. This makes it a very common choice for example in diagnostic applications, or in situations with imbalanced classes. For each feature $X_j$, we use the following prediction rule of the binary response variable $Y$: $\hat{Y} = \mathbb{I}_{c,\infty}(X_j)$, with $\mathbb{I}$ denoting the indicator function. That is, if $X_j$ is greater than a certain threshold $c$, we predict class 1. Otherwise, class 0 is predicted. The Receiver Operating Characteristic curve displays the sensitivity and specificity of this classification rule for all choices of $c$. The area under this curve defines a trade-off measure of both aspects and is hence often used to assess the overall quality of a prediction rule. For this measure, a value of 0.5 corresponds to a random prediction and values of 0 and 1 denote a perfect separation of the class variable. We define a monotonous version of the AUC by

$$J_{\text{AUC}}(X_j) = 2 |\text{AUC}_{\hat{Y}}(X_j) - 0.5|,$$

which transforms the value of a random prediction to 0 and a perfect separation to 1. To introduce a cost-sensitive version of this measure, a benefit-cost ratio approach similar to Equation (1) is used. For each feature $X_j$ with feature cost $c_{X_j}$, the
benefit-cost ratio measure for AUC filtering is given by

$$\text{BCR}_{\text{AUC}}(X_j, \xi) = \frac{J_{\text{AUC}}(X_j)}{c^{\xi X_j}}.$$  \hspace{1cm} (3)

where $\xi$ is a hyperparameter to control the trade-off between performance and cost. We compare different strategies for this hyperparameter in the simulation study in Section 3.

After obtaining an individual BCR value for each feature, a top-down approach is used to built up a feature set that meets the budget limit. Features are added to the result set in order of their $\text{BCR}_{\text{AUC}}$ rank, but only, if the cost of the resulting model does not exceed the budget. The process is stopped, when the cost of any remaining feature would exceed the budget (Jagdhuber et al., 2020).

2.3 Feature Filtering by Permutation Feature Importance (pFI)

Another popular approach particular to Random Forests is the permutation Feature Importance (pFI) (Breiman, 2001). It is a heuristic measure, which assesses the relevance of individual features in a full Random Forest model. To calculate this measure, the observations of a single feature $X_j$ are permuted and the OOB error of the resulting Random Forest is computed. As the permutation removes any predictive information of the variable $X_j$, the difference of this OOB error to the original one describes a measure of importance for $X_j$. This measure has both univariate and multivariate aspects. On the one hand, the score of a feature is based on the multivariate context of a Random Forest model and could thus be labeled multivariate. On the one hand, each feature is assigned an individual score, which is then typically used for a one-by-one feature selection. As relevant combinations may be separated, a high importance value does not necessarily imply a good performance in a smaller subset of features.

We label the permutation feature importance measure $J_{\text{pFI}}(X_j)$. It can take values between 0 and 1, with larger values corresponding to a higher importance of the respective feature. Similar to the AUC, we propose a cost-sensitive version of this measure with

$$\text{BCR}_{\text{pFI}}(X_j, \xi) = \frac{J_{\text{pFI}}(X_j)}{c^{\xi X_j}}.$$  \hspace{1cm} (4)

where $\xi$ is a hyperparameter to control the trade-off of performance and cost. To built up a final result set from the individual feature assessments, the same approach as described in Subsection 2.2 is used.

2.4 Random Forest Forward Selection

The third additional approach of this paper introduces a common feature selection strategy found for example in linear models for the context of Random Forests. A greedy sequential Forward Selection (FS) starts with an empty set of features and iteratively adds the one feature that best extends the current result set. Best is typically defined by means of goodness of fit, or predictive performance. In our context, this translates to building a Random Forest model for each candidate set and assessing the respective OOB errors. The central problem of this approach is the high computational complexity of Random Forests in general associated with the large number of models needed. Consider a setting with 1000 features. In the first iteration, the forward selection grows and assesses 1000 (one feature) Random Forests. In the second iteration there are 999 Random Forests to be evaluated. After 100 iterations, a total of 95050 models needs to be computed. The only exception to this would be situations with small budgets, where many paths could be eliminated early on. For all other problems, however, the computational effort of this method can be immense. Even with fast implementations, like for example found in the R package ranger (Wright and Ziegler, 2015), the overall run-time is hard to manage in practice.
Nevertheless, we implemented this approach for our analyses in a cost-constraint context. At iteration \( k \), the forward selection needs to decide which feature \( X_j \) is added to the current result set \( S \). We propose the following cost-sensitive criterion for this decision:

\[
\text{BCR}_{\text{FS}}(X_j, S_k, \xi) = \frac{\text{MMCE}_{\text{OOB}}(\text{RandomForest}((S_k \cup X_j))) - \text{MMCE}_{\text{OOB}}(\text{RandomForest}((S_k)))}{(c_{(S_k \cup X_j)} - c_{(S_k)})^{\xi}} \tag{5}
\]

The stopping criterion and the decision on a final solution follow the ideas discussed in Subsection 2.1.3. Similar to the previous sections, Equation (5) introduces a hyperparameter \( \xi \) to control the trade-off of cost and performance. Tuning this hyperparameter requires to execute the feature selection process for a reasonable set of candidate values. With the immense run-time of each FS run, this was not feasible for the simulation setup of Section 3. Our most promising attempt used a model-based optimization approach, which however still required approximately 10 hours for the tuning process of one simulation run. Therefore, we do not consider hyperparameter tuning for FS and only assess the cost-agnostic and the simple BCR strategy in the following.

3 Simulation Study

The structure of this section follows ADEMP, a framework proposed by Morris et al. (2019) to systematically define simulation studies. ADEMP is an acronym for: Aims, Data-generating mechanisms, Estimands, Methods, Performance measures. In the following, we address each element of ADEMP in an individual section to provide a thorough outline of all performed analyses.

3.1 Aims

Our simulation study evaluates feature selection methods for Random Forest classification tasks in a cost-sensitive setup. We do not intend to claim a general best method for all situations, but rather to understand strengths and weaknesses of the analyzed methods in realistic data settings. Additionally, we compare different strategies for our BCR criterion to assess the impact of a hyperparameter controlled trade-off approach compared to more simple strategies. In summary, the simulation study addresses the following main questions:

1. Is there a general benefit from using a simple BCR approach (\( \xi = 1 \)) in the proposed methods instead of a cost agnostic strategy (\( \xi = 0 \))? If not, is there any other globally best setting for \( \xi \)?
2. Does the hyperparameter tuning approach for \( \xi \) generate a relevant improvement compared to the alternatives discussed in Aim 1?
3. Which of the analyzed methods show strengths/weaknesses for data simulated with only univariate effects on a binary response variable? Which do so for multivariate effects?
4. Does the extent of the budget constraint \( c_{\text{max}} \), or a correlation between cost and relevance of a feature affect these results?
5. Can we observe similar or further effects when applying the proposed methods on real-world data?
6. Can the proposed methods outperform their respective cost-agnostic baseline versions on real data?
7. Can we categorize strengths and weaknesses of each method by the known meta information of the data sets?

After presenting the simulation results in Section 4, a detailed step-by-step discussion of each aim is provided in Section 5.

3.2 Data-generating mechanism

The simulation study is divided into two parts. The first part analyzes four settings on artificially generated data, while the second part evaluates six real-world data sets. In this section, we describe the processes to generate all artificial data sets and provide background information on the origins of the real-world data sets.
3.2.1 Artificial Data Settings

For the artificial simulation settings, we consider data sets of \( n_{\text{obs}} = 500 \) observations with \( p = 200 \) continuous numeric features, representing a typical set-up for example in metabolomic studies or phase-III trials (Banas et al., 2018). Data sets are generated following the framework of Boulesteix et al. (2017). First \( n_{\text{obs}} \) realizations of the binary response variable are drawn from the Bernoulli distribution \( \mathcal{B}(0.5) \). After that, the corresponding features to each response value are drawn from the \( p \)-dimensional normal distributions

\[
X_1, \ldots, X_p \mid Y = 1 \sim N_p(\mu, \Sigma),
\]

\[
X_1, \ldots, X_p \mid Y = 0 \sim N_p(0, \Sigma),
\]

with mean vector \( \mu \) defined as

\[
\mu^T = (\beta_1, \ldots, \beta_{p_{\text{rel}}}, 0, \ldots, 0).
\]

To include a variety of weak, mediocre and strong effects, we draw the \( p_{\text{rel}} = 100 \) realizations of \( \beta_j, j = 1, \ldots, p_{\text{rel}} \) from a truncated normal distribution \( N_{[-1,1]}(0,0.5) \). This truncated normal distribution can be interpreted as a usual normal distribution, where only realizations within the interval \([-1, 1]\) are considered valid. We thus avoid unrealistically dominant effects. The remaining elements of \( \mu \) are set to zero, and the corresponding features can be interpreted as noise.

For the covariance matrix \( \Sigma \), we consider two alternatives. The first choice represents a scenario of independent features with only univariate relations to the response variable. This assumes \( \Sigma = I_p \) and is labeled “Independent Data”. In many real-world applications, however, the assumption of completely independent features does not hold true (De Meyer et al., 2008). Therefore, we also consider a scenario with “Correlated Data”, i.e. a non-diagonal covariance matrix \( \Sigma \). More specifically, we assume 20 groups of mutually correlated features, which corresponds to the following block-diagonal covariance matrix:

\[
\Sigma = \begin{pmatrix}
S(\rho_1) & 0 & 0 \\
0 & \ddots & 0 \\
0 & 0 & S(\rho_{20})
\end{pmatrix},
\]

where \( S(\rho_i), i = 1, \ldots, 20 \) is a \( \frac{p^2}{2} \times \frac{p^2}{2} \) matrix with ones on the diagonal and \( \rho_i \) outside the diagonal. Realizations of \( \rho_i \) are drawn from the uniform distribution on the interval \([0, 1]\). By only considering positive values for \( \rho_i \), we can ensure that \( \Sigma \) is positive definite. To randomly distribute informative features (i.e. the non-zero entries of \( \mu \)) and noise features across this correlation structure, the order of the features in this matrix is permuted, permuting columns and rows of \( \Sigma \) at the same time, before drawing from \( N_{\Sigma}(\cdot, \Sigma) \). One goal of defining a non-diagonal covariance matrix is to create a multivariate modelling problem. It may not seem obvious that correlated features automatically correspond to multivariate effects on the response variable. However, with the data-generating mechanism of Equation (6) any pair of correlated features with non-identical effect sizes induces an additional separation that is proportional to the extent of the correlation (cf. Figure 2 of Jagdhuber et al. (2020)). Note that this consequently also changes the interpretation of the defined effect sizes in Equation (7).

In these settings, the absolute size of \( \beta \) does not define the relevance of the respective feature anymore and therefore a feature with effect size zero can no longer generally be seen as noise. However, as we avoid interpretations concerning, e.g., the number of detected relevant and noise features, this does not affect the analyses in the following.

For the feature costs \( c_j, j = 1, \ldots, p \), we also consider two alternatives. In the first scenario (labeled “Independent Costs”), feature costs are drawn from a uniform distribution on the interval \([0, 1]\). This assumes that costs \( c_j \) are independent of the respective effect sizes \( \beta_j \). In practice, it can also be plausible to assume that more valuable features might be more expensive on average. We therefore consider a scenario of “Correlated Costs” as well. In this scenario, the cost of the \( j \)-th feature is computed using the absolute value of \( \beta_j \) and adding normal distributed uncertainty to it. After that, the value is truncated to our intended cost range \([0, 1]\). Formally this can be written as

\[
c_j = \min(1, \max(0.1, |\beta_j| + \epsilon_j)),
\]
where $\epsilon_j \sim N(0, 0.2)$. For the overall budget limit $c_{\text{max}}$ we consider five values, which represent small, medium and large budgets, by defining $c_{\text{max}} \in \{1, 2, 5, 10, 30\}$.

Altogether, two scenarios for the choice of $\Sigma$ and two scenarios for feature cost correlations are varied and each setting is evaluated at five feature cost budget limits. To thoroughly analyze all possible effects, we use a factorial design resulting in four settings named A to D with five budget limits each. An overview of these settings is given in Table 1.

All methods are applied on a set of $n_{\text{sim}} = 100$ training data sets, which are drawn as follows: In a first step, a fixed value for $\mu$, which is used in all settings A to D, and the block-diagonal matrix $\Sigma$ of Definition 8, which is used for settings C and D, are drawn. Furthermore, a set of independent costs for settings A and C and a set of correlated costs for setting B and D are generated. With these elements, $n_{\text{sim}} = 100$ training data sets with $n_{\text{obs}} = 500$ observations and one test data set with $n_{\text{max}} = 5000$ observations are drawn respectively for the independent and correlated settings according to the framework described above in this section. The analysis of these data sets is structured into the following steps. All methods are applied to the training data sets for a grid of values $\xi$ including $\xi = 0$ and $\xi = 1$. Among these grid values, the resulting feature sets at $\xi = 0$ (cost-agnostic results), $\xi = 1$ (simple BCR results) as well as the set with the lowest OOB error (hyperparameter tuning results) are selected for every feature selection method. These sets are used to build full Random Forest models on the training data, which are then evaluated on the test data set to obtain the MMCE.

3.2.2 Real-World Data Settings

In addition to the artificial simulations, we also include a real-world study in our analyses. The online platform Open-ML (Vanschoren et al., 2013) provides a large collection of well documented data sets that can be filtered by relevant meta-information like the number and type of features, the response variable type, the amount of missing values and more. For the objectives of this paper, six binary classification data sets met all requirements, which included a sample size of at least 500 observations, no missing values, and a total between 30 and 500 non-categorical features. We aimed to select data from many different fields to cover a large variety of practical applications. The exception to this is image analysis, as a setup of different feature costs for individual pixels seems unreasonable. An overview of all real-world data sets used in this paper is given in Table 2. A short introduction on every data set is provided in the following.

### Table 1

| Setting   | Data Covariance $\Sigma$ | Relationship $\beta_i \sim c_i$ | Cost budget limit $c_{\text{max}}$ |
|-----------|--------------------------|---------------------------------|-----------------------------------|
| Setting A | Independent Data         | Independent Costs               | $\{1, 2, 5, 10, 30\}$            |
| Setting B | Independent Data         | Correlated Costs                | $\{1, 2, 5, 10, 30\}$            |
| Setting C | Correlated Data          | Independent Costs               | $\{1, 2, 5, 10, 30\}$            |
| Setting D | Correlated Data          | Correlated Costs                | $\{1, 2, 5, 10, 30\}$            |

### Table 2

| Data Set  | $p$ | $n_{\text{obs}}$ | $P(y = 1)$ | Field            | Source                        |
|-----------|-----|-----------------|------------|------------------|-------------------------------|
| Ada       | 48  | 4562            | 0.248      | Social Studies    | https://www.openml.org/d/40993 |
| Author    | 70  | 841             | 0.377      | Text Mining       | https://www.openml.org/d/1481  |
| Qsar      | 41  | 1055            | 0.337      | Biology           | https://www.openml.org/d/1494  |
| Spam      | 57  | 4601            | 0.394      | Text Mining       | https://www.openml.org/d/44     |
| Tokyo     | 44  | 959             | 0.639      | Server Performance| https://www.openml.org/d/40705  |
| Wdbc      | 30  | 569             | 0.373      | Medicine          | https://www.openml.org/d/1510  |

In addition to the artificial simulations, we also include a real-world study in our analyses. The online platform Open-ML (Vanschoren et al., 2013) provides a large collection of well documented data sets that can be filtered by relevant meta-information like the number and type of features, the response variable type, the amount of missing values and more. For the objectives of this paper, six binary classification data sets met all requirements, which included a sample size of at least 500 observations, no missing values, and a total between 30 and 500 non-categorical features. We aimed to select data from many different fields to cover a large variety of practical applications. The exception to this is image analysis, as a setup of different feature costs for individual pixels seems unreasonable. An overview of all real-world data sets used in this paper is given in Table 2. A short introduction on every data set is provided in the following.
Ada. The main task of ADA is to identify citizens with high revenue. This is a two-class classification problem. The raw data from the census bureau is also known as the “Adult” database in the UCI Machine-Learning Repository (Dua and Graff, 2017). The 14 original features include age, work-class, education, marital status, etc., but are pre-processed and scrambled into a 48 feature continuous numeric representation (Goschenhofer, 2017).

Author. The original version of this data set is part of a collection of data sets used in the book “Analyzing Categorical Data” by Simonoff (2013). The categorical response variable consists of the author labels “Austen”, “London”, “Milton” and “Shakespeare”. Features correspond to word frequencies of 70 different words. The data set used in this paper is a binarized version of the original set, where the response variable is converted by re-labeling the majority class (“Milton”) as 1 and all others as 0.

Qsar. The QSAR biodegradation data set (Mansouri et al., 2013) was built in the Milano Chemometrics and QSAR Research Group. The data have been used to develop QSAR (Quantitative Structure Activity Relationships) models for the study of the relationships between chemical structure and biodegradation of molecules. A total of 1055 chemicals result in 41 numeric molecular descriptor features and one binary response variable with classes ready biodegradable and not ready biodegradable.

Spam. A data set of Hewlett-Packard Labs containing 4601 E-mails together with a user based classification into “Spam”, or “No Spam”. Features include word and character frequencies as well as further general numeric measures on the text composition (Dua and Graff, 2017).

Tokyo. Performance-Co-Pilot (PCP) data for the Tokyo server at Silicon Graphics International. The data characterizes the server performance as either “good” (1) or “bad” (0). The 44 numeric features include technical measures like the average percentage of CPU time spent for user code, read and write rates, or average free memory. The instances are measurements generated by the PCP software every five seconds.

Wdbc. The Wisconsin Diagnostic Breast Cancer data set describes characteristics of cell nuclei from a digitized fine needle aspiration procedure (FNA) of a breast mass. Ten real-valued features are computed for each of three cell nuclei, yielding a total of 30 descriptive features. These features include for example radius, smoothness, and symmetry. The response variable records the prognosis as either “benign” (0) or “malignant” (1).

In their original form, none of these real-world data sets includes feature costs. Therefore, a cost setting analogous to the “Independent Costs” scenario of the artificial data is simulated. As the true effects of features are not simulated and estimations of these require strong and possibly unrealistic assumptions, we do not generate a “Correlated Costs” scenario here. Instead, all feature costs are drawn from the uniform distribution on the interval $[0, 1]$. To also analyze possible effects of this random draw, for the Spam data set, we define five different cost vectors and compare the obtained results. As the number of relevant and total features varies between data sets, the feature cost budget limits are chosen individually. For each data set, five candidates representing a range of small to very large constraints are analyzed.

Furthermore, the real-world data sets are not split into training and testing sets. Thus, we create these splits manually. $n_{\text{sam}} = 100$ random split points, which partition data sets into $\frac{2}{3}$ of observations to be used as training sets and $\frac{1}{3}$ of observations to be used as testing set are defined. The analysis itself is structured similarly to the artificial settings. All methods are applied for a grid of $\xi$ values to each of the training partitions. Among these grid values, the resulting feature set at $\xi = 0$ (cost-agnostic baseline) and the set with the lowest OOB error (hyperparameter tuning results) are selected. These sets are used to build full Random Forest models on the training partitions, which are then evaluated on the test partitions to obtain the MMCE.

3.3 Estimands and Targets

Our statistical analysis task is to select a feature subset from a pool of candidate features and then predict a binary response variable with a Random Forest model. First, the feature selection and Random Forest model fit are performed on training data. This model then predicts the response variable of an independent test data set. In the sense of Morris et al. (2019), this response variable represents our final estimand and the respective predictions of each candidate model can be seen as the target of the analysis.
3.4 Methods

The simulation study analyzes methods for feature selection in binary Random Forest classification problems. The compared methods are:

- **STS**: Shallow Tree Selection (see section 2.1).
- **AUC**: AUC Filter (see section 2.2).
- **pFI**: Permutation Feature Importance (see section 2.3).
- **FS-0**: Forward Selection with $\xi = 0$ and
- **FS-1**: Forward Selection with $\xi = 1$ (see section 2.4).

Besides the comparison of feature selection methods, further interest lies in the analysis of strategies for the hyperparameter $\xi$. We compare a **cost-agnostic strategy** with a fixed value $\xi = 0$, a **simple-BCR strategy** with a fixed value $\xi = 1$ and a **hyperparameter tuning strategy** with an adaptively optimized value $\xi$ based on Grid Search. An introduction of these strategies is given in Subsection 2.1.2. For the real-world simulations, the cost-agnostic versions define the baselines for each of the proposed methods, respectively.

3.5 Performance Measure and Monte Carlo SE

The MMCE of a Random Forest model (no individual parameter tuning; num.trees = 1000, mtry = $\sqrt{p}$) applied on independent test data is used to summarize and assess the selected feature sets. For a global comparison of all methods and strategies described in the previous sections, the mean of the MMCEs over the 100 simulation runs is taken. This value represents our final performance measure for each method and is labeled MMCE in the following. As comparisons of this measure can only be assessed in the context of the simulation setup, we consider the uncertainty in terms of the Monte Carlo standard error. An approximate estimate of the Monte Carlo standard error (SE) of MMCE is given by

$$\text{Monte Carlo SE}(\text{MMCE}) = \sqrt{\frac{\text{Var}(\text{MMCE})}{n_{\text{sim}}}}.$$  \hspace{1cm} (10)

A two-sided $\alpha$-level confidence interval for MMCE can thus be written as

$$\text{CI}_{\alpha}(\text{MMCE}) : \left[ \text{MMCE} \pm q_{1-\frac{\alpha}{2}} \cdot \text{Monte Carlo SE}(\text{MMCE}) \right],$$ \hspace{1cm} (11)

where $q_{1-\frac{\alpha}{2}}$ is the $(1 - \frac{\alpha}{2})$-quantile of the standard normal distribution.

With regard to the individual run-times of all methods and the factorial design of the study, the definition of $n_{\text{sim}} = 100$ provides an acceptable reduction of uncertainty at a feasible computational effort. To account for this uncertainty, all following results comparing MMCE values are reported with their respective 95%-confidence intervals as defined in Equation (11). Additionally, all individual Monte Carlo standard errors for every setting, budget limit and method are tabulated and can be found in Additional file 1.

4 Results

4.1 Artificial Data Results

The first analysis focuses on the proposed BCR criterion of each method. For all hyperparameter configurations, the MMCE on the test data set is computed. An exemplary overview of the results is given in Figure 3 for setting D with budget limit 10. This setting was chosen as it shows many characteristics also found in the other settings of the factorial design. Corresponding illustrations for every setup can be found in Appendix 6.
Fig. 2 Three plots with two subplots each corresponding to the analyzed feature selection methods using the BCR criterion. Each left subplot shows a colored line of connected points representing the mean MMCE over all 100 simulation runs at a grid of \( \xi \) values. The dark-shaded ribbon represents a 95%-CI around this mean value. The light shaded area shows the region between the 5% and 95% quantiles of the empirical distribution of the MMCE. The mean MMCE at \( \xi = 0 \) and \( \xi = 1 \) are highlighted with a gray and an orange point, respectively. Each right subplot shows violin plots of the empirical MMCE distributions for the analyzed hyperparameter strategies. The 95%-CI region of the mean is given by a black box over the violins. Finally, the mean MMCE values of the three strategies are annotated with dashed lines over both subplots. Note that the hyperparameter tuning strategy (green) does not correspond to a single point on the left subplots, as \( \xi \) is chosen at each simulation run independently of the OOB error of the current model. This plot shows results for setting D with \( c_{\text{max}} = 10 \). Corresponding plots for all other levels of the factorial design are given in Appendix [6].

All resulting curves of Figure 2 are convex, i.e. with larger values of \( \xi \) the MMCE values first decrease and after a certain point begin to increase again, eventually exceeding the initial MMCE value at \( \xi = 0 \). This trend is also observed in almost all other analyzed settings. The only exceptions to this is STS for setting C, with \( c_{\text{max}} = 2 \) and \( c_{\text{max}} = 5 \), where the minimum occurs at \( \xi = 0 \) and MMCE values increase from there on. When comparing the cost-agnostic and the simple BCR strategy, none is generally superior for all settings. In Figure 2 the results already differ greatly between methods. The cost-agnostic strategy is superior for AUC, the simple BCR strategy is superior for pFI and both are approximately equal for STS. This uncertainty is also observed for other settings with no general preference for either of both strategies. Furthermore, the actual minima of the curves do not tend towards any fixed value, but also differ over all analyzed settings and methods. An alternative to defining a fixed \( \xi \) is given by the hyperparameter tuning strategy, which selects a separate value of \( \xi \) in each simulation run. With this adaptive strategy, the tuning approach is able to produce generally lower mean MMCE values than any point on the curves. In the majority of settings, hyperparameter tuning resulted in notably lower mean MMCE values compared to the cost-agnostic and simple BCR strategies. With larger budget values, differences between strategies decrease on an absolute scale, yet remain similar relative to the Monte Carlo SE of the MMCEs. The data and cost-correlation definitions of settings A to D showed no further effects.

In all following method comparisons we focus on simulation results of the hyperparameter tuning strategy for AUC, pFI and STS and omit the inferior cost-agnostic and simple BCR strategies. To compare the proposed feature selection methods for every level of the factorial simulation design, a comprehensive illustration of all MMCE results is given in Figure 3.

The first two rows of this figure illustrate the independent data settings A and B. In these settings, the univariate filter method AUC shows the lowest mean MMCE closely followed by pFI. STS comes in third with significantly larger mean MMCE values. Here, and in the following, “significant” refers to the (unadjusted) 95%-Monte Carlo SE confidence intervals of the mean MMCEs. We conservatively consider two methods to differ significantly, if two CIs do not overlap. The worst performances are observed for FS-0 and FS-1, where similar to the results of the hyperparameter strategy analysis, none of both is generally superior. For the correlated data settings C and D, the method rankings differ notably. In most situations
STS significantly outperforms the alternative methods. Among the FS methods, FS-1 generally shows lower mean MMCE values compared to FS-0 here. Yet, in almost all cases both cannot compete with pFI and STS. The same applies to AUC, which also typically appears at the bottom end of the ranking. For all settings A to D, increasing the size of the budget limit results in smaller absolute differences between methods. In settings C and D, differences relative to the Monte Carlo SE of the MMCEs also slightly decrease with higher budget limits. This effect is, however, not notable in settings A and B.
Correlation of feature relevance and costs revealed no obvious effects in our results. Altogether, the main influencing factor of the performance ranking in our artificial simulation is if independent or correlated data are present.

4.2 Real-World Data Results

As the data correlation notably influenced the results of the artificial simulation, our first analysis of the real-world data concerns the correlation between the features. Boxplots of the absolute correlation values observed in the six real-world data sets and corresponding boxplots for the artificial settings are given in Figure 4.

![Boxplots for the absolute correlation values of all real-world data sets. Additionally, correlation boxplots for the block-diagonal matrix of Equation 8 used in the artificial simulation are shown (first two lines), including also zeros (all) and including only non-zeros (> 0).](image)

To highlight the design of the artificial simulations, the block-diagonal structure of $\Sigma$ in Equation 8 is illustrated in two versions. The first version, which includes all values, shows that only very few actually correlated entries are found in $\Sigma$. However, these non-zero entries cover a large range, which is illustrated by the second boxplot. The observed real-world correlations differ from this structure. Ada and Spam contain rather small correlations with an average around 0.1. Compared to these, the boxplots of Author, Qsar and Tokyo include notably higher correlations and have their mean at approximately 0.2. The highest correlations are found at Wdbc, with multiple strong correlations above 0.9 and a mean of approximately 0.4.

The main aim of the real-world simulation is a comparison of the proposed methods for every analyzed data set and budget limit. To illustrate these results in a comprehensible format, we depict the main performance criterion (MMCE) together with its respective 95%-Monte Carlo CI for all setups. A large plot-matrix of these results can be found in Appendix 6. An overview of the main results from representative setups is given in Figure 5.

Altogether, the results vary strongly between different setups. Each non-baseline method significantly dominates the other methods in at least one of the setups. Examples of such “best” methods are: AUC for Qsar with $c_{\text{max}} = 1$, FS-1 for Wdbc with $c_{\text{max}} = 1$, pFI for Spam with $c_{\text{max}} = 5$, and STS for Author with $c_{\text{max}} = 1$. The latter two are also illustrated in Figure 5. Method rankings do not only vary between different data sets, but also change for different budget limits. For Spam, for example, the best method changes along four of the five analyzed budget limits, see Appendix 6. Similar to the artificial data, differences between methods and the size of the CIs decrease with increasing budget. For the Spam data, we also analyzed effects of different random draws of the cost vector by sampling 5 versions of this vector. Detailed plots of the individual results for each random draw can be found in Appendix 6. While a general tendency to favor pFI can be observed for most Spam data versions, the analysis shows that different rankings can also arise from different explicit cost setups. Comparing the results with respect to the correlations shown in Figure 4, no notable associations can be observed. For Qsar, which has
Fig. 5  Top: Method comparison results of three representative real-world data sets and budget limits $c_{\text{max}}$. Crosses show the mean MMCE for each feature selection method, and horizontal bars show the corresponding 95%-Monte Carlo confidence intervals of these means. The cost-agnostic baseline version of each method is highlighted by adding "-0" to its name. Bottom: Mean rank of each method over all analyzed real-world simulation settings. Methods on the y-axis are sorted by mean rank.

relatively high correlations, the univariate AUC method performed best. On the contrary, the relatively weak correlations of Ada favored more multivariate-oriented methods like FS and STS. Both showed weaknesses for non-correlated data in the artificial simulations. When categorizing the data sets by their field according to Table 2, no obvious groups can be found as well. Author and Spam, for instance, both originating from a similarly structured text mining application, both benefit from completely different methods. While individual rankings may vary for different setups, a clear overall preference for non-baseline methods is notable in almost all setups.

To obtain a global measure of the simulation results, the average rankings of each method over all analyzed data sets (excluding the cost-vector repetitions of Spam) are illustrated in the bottom plot of Figure 5. This plot shows that on average the whole group of baseline methods ranks worse than all non-baseline methods. Within the non-baseline methods, STS and pFI furthermore show an improvement of almost a full rank on average. Altogether, while local differences highlight that no universally superior method exists for all setups, the global rankings show notable preferences towards non-baseline approaches, specifically STS and pFI.

5 Discussion

With the results presented in the previous section, we address all aims defined in Section 3.1 as follows. Aim one concerns the hyperparameter in the BCR criterion (see Section 2.1.2) and compares the proposed cost-agnostic and simple BCR strategies. The results in Figure 2 show that there is no generally superior strategy with a fixed value for $\xi$. That means, not only the proposed strategies, but also other possible choices for $\xi$ are unsuited as a general solution for different data sets or even different budget limits within a single data set.
Aim two extends this topic by evaluating the benefits of a hyperparameter tuning strategy. In almost all simulations, this strategy notably improved the overall feature selection results. By not defining a global value $\xi$, but selecting the optimal value for each simulation run independently, hyperparameter tuning outperformed any fixed $\xi$ approach. As the additional computational complexity does typically not create run-time issues for fast methods like AUC, pFI or STS, we therefore generally recommend to use hyperparameter tuning for these approaches.

The third aim analyzes strengths and weaknesses of methods on univariate and multivariate data sets. The univariate case corresponds to the results of the artificial settings A and B. Here, AUC generally provides strong results. This seems reasonable, as the theoretical idea of a univariate filter exactly targets the simulated data scenario. STS, which focuses on multivariate tree structures, shows some weakness at purely univariate setups. While FS is also notably inferior here, we avoid general conclusions on this method, as it uses the inferior cost-agnostic and simple BCR strategies. pFI handles the data structure similarly to AUC and can thus also be considered well suited for univariate settings.

The multivariate data case corresponds to the artificial settings C and D. Here, STS outperforms the other methods in almost every setup. While the multivariate nature of these settings emphasizes the weaknesses of STS, it also exposes the main weakness of AUC, which as a univariate filter approach is not able to identify the relevant structures and clearly falls behind here. pFI ranks features by their importance in a Random Forest fitted on all features. The multivariate aspect of this approach renders it superior to AUC. However, for most of the analyzed setups, filtering by this importance measure is inferior to the procedure of STS, which evaluates smaller, but coherent combinations. Nevertheless, pFI still provides the second best alternative here and can be considered well-suited as well. Method rankings of FS are inconsistent and vary between setups.

Aim four concerns effects of different budget limits $c_{\text{max}}$, and possible influences from a correlation of true feature effect sizes and feature costs. In some artificial and real-world settings, larger budgets reduce the differences between approaches and the actual method choice becomes less relevant. This does however not hold true in general. In many real-world data sets, the best method changes for different budget limits. Nevertheless, there is no notable systematic preference of methods for small or large budgets. Besides these mentioned aspects, no further budget effects are observed. The same applies to the analyses on correlated effect sizes and feature costs. While this setup defines a realistic scenario, which in most simulations influences the selection of the features, it does not affect the method comparison results in any major way.

The fifth aim addresses further effects detected on real-world data that extend the findings of the artificial simulations. From the real-world results we conclude that our artificial design is only able to tackle a few aspects of the actual data generating process of many real-world data sets. The individuality of the results hints towards many unknown factors, which further influence the suitability of a method. However, these aspects cannot be specified from the data at hand and would require further detailed research.

Aim six focuses on the comparison to the baseline methods in the real-world analysis. Results of nearly all individual setups show that the baseline versions of all methods are inferior to their non-baseline counterparts. A global analysis of the average rankings of each method furthermore highlighted that even the lowest ranking non-baseline method (AUC) ranks above the best baseline method (FS-0). Therefore, we conclude that the proposed methods outperformed the cost-agnostic baseline approaches.

The final aim considers categorizing method preferences of real-world data sets according to given Metadata. We could not identify common factors of the real-world data sets that lead to a preferred method. Moreover, the results show evidence that local differences in the highest ranking method can already arise from different budget limits or explicit cost definitions. On a global level, however, an analysis of average method rankings shows that STS and pFI are more versatile than other methods and on average rank notably higher.

6 Conclusion and Outlook

Our paper proposed multiple methods for cost-sensitive feature selection in the context of Random Forests. The first of these is a novel approach named STS. STS identifies a set of relevant small tree structures from an ensemble of candidate trees and selects the minimal feature subset that is able to build these structures. It thus provides a computationally efficient solution for a multivariate feature selection problem. Besides STS, we also proposed three further adaptations of common feature selection approaches for Random Forests. With AUC as a univariate filter approach, pFI as a semi-multivariate approach and
FS as a true multivariate, but computationally complex approach, a diverse set of methods was defined for the problem at hand. In a large scale simulation study of four artificial data settings and six real-world data sets, strengths and weaknesses of all methods were assessed. There is no universal one-fits-all method among our candidates. Each approach was superior in at least one of the analyzed settings. This illustrates the fundamental differences in the basic selection strategies of each algorithm, which can be more or less suited in different data situations. The factors guiding the optimality of a method may, however, often depend on possibly unknown data generating mechanisms. For each method, an individual use-case setting could be found in our simulation. A global analysis of the rankings of each method over all data sets nevertheless showed that STS and pFI on average ranked notably higher than their competitors and may thus be considered favorable candidates in unknown situations. Nevertheless, for a practical problem, we still recommend applying multiple methods (e.g. the computationally fast AUC, pFI and STS approaches) and base a final decision on a comparative analysis. If the high complexity of FS is manageable for the problem at hand, we recommend to also include this approach. Regardless of the method, all BCR approaches discussed in this paper highly benefited from a hyperparameter tuning, and we therefore finally advise to ensure an adequate trade-off of performance and cost with a hyperparameterized BCR criterion.

Beyond the developments in this paper, in the following we mention a few further ideas for future research on this topic. In the current implementation of STS, the number of features per tree is limited by the tree depth. This is a practical solution, which has multiple downsides. First, a limited depth generally reduces predictive performance. Second, this approach does not guarantee that exactly the intended number of different features per tree is selected. An alternative to limiting the tree depth could be to limit the number of features a tree may use instead and allow the tree to fully grow. For example, if we intend to build a three-feature tree, the tree-growing algorithm may perform normal splits until three distinct features have been used. From then on, it may continue to perform further splits, but only with these three features. Instead of limiting the number of features, limiting the cost of the tree itself might be another viable option. This would extend the set of candidate trees even further. Moreover, trees could also be generated in a cost-sensitive manner that includes a trade-off between costs and performance at each split.

In the STS method described in this work, the base ensemble of trees is generated from a Random Forest framework. However, it should be noted that any tree growing algorithm generating heterogeneous trees may be used instead. With a more general approach, redundant trees could be avoided or special multivariate structures could be emphasized. For future analyses, alternative strategies for the hyperparameter tuning – apart from a simple Grid Search – might increase performance and reduce the run-time of all methods. Especially for FS, such developments may be a relevant aspect deciding if the method is feasible at all. Finally, all current simulations specialize on binary classification. Yet none of the proposed methods is technically limited to this setup. Analyzing the effects on different response and model types therefore also provides a good basis for further research in this field.

Appendix

Additional file 1

Table of all Monte Carlo standard errors. (PDF)
Monte Carlo SE estimates of the mean MMCE after \(n_{\text{sim}} = 100\) simulation runs. The table shows estimates for all analyzed methods, budget limits and data sets of the simulation study of this paper.

Additional file 2

Comprehensive version of Figure 2 including all levels of the factorial design for the artificial data simulation. (PDF)
Each full figure illustrates a certain setting and budget limit combination. Details on the individual elements of these figures can be found in the description of the analogously structured Figure 2.
Additional file 3

Plot matrix of all analyzed real-world data sets (rows) and budget limits $c_{\text{max}}$ (columns). (PDF)

Crosses show the mean MMCE for each feature selection method. Horizontal bars show the corresponding 95%-Monte Carlo confidence intervals of these means. Methods on the y-axis are given in increasing order of mean MMCE to provide a visual ranking for each simulation setup. The cost-agnostic baseline version of each method is highlighted by adding “-0” to its name.

Additional file 4

Plot matrix of the Spam data results for five random draws of the cost vector. (PDF)

Crosses show the mean MMCE for each feature selection method. Horizontal bars show the corresponding 95%-Monte Carlo confidence intervals of these means. Methods on the y-axis are given in increasing order of mean MMCE to provide a visual ranking for each simulation setup. The cost-agnostic baseline version of each method is highlighted by adding “-0” to its name.

Declarations

Funding

This work was supported by Deutsche Forschungsgemeinschaft (DFG), Project RA 870/7-1, and Collaborative Research Center SFB 876, A3. The authors acknowledge financial support by Deutsche Forschungsgemeinschaft and Technische Universität Dortmund within the funding programme Open Access Publishing.

Conflict of interest

The authors declare that they have no conflict of interest.

Availability of data and material

All data sets and material used in this paper are available on Github: https://github.com/RudolfJagdhuber/STS

Code availability

The full code used in this paper is available on Github: https://github.com/RudolfJagdhuber/STS

Authors contributions

Rudolf Jagdhuber, developed all methods, designed and executed the simulation studies, interpreted the results, and wrote the manuscript. Michel Lang proposed the first idea of Tree Selection and corrected and approved the manuscript. Jörg Rahnenführer initiated the topic, supervised the project, contributed to the problem definition, the design of the simulation study and to the interpretation of the results, and corrected and approved the manuscript.
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