Approaches for Rule Discovery in a Learning Classifier System

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- Keywords: Rule Set Learning, Rule-based Learning, Learning Classifier Systems, Evolutionary Machine Learning, Interpretable Models, Explainable AI.
- Abstract: To fill the increasing demand for explanations of decisions made by automated prediction systems, machine learning (ML) techniques that produce inherently transparent models are directly suited. Learning Classifier Systems (LCSs), a family of rule-based learners, produce transparent models by design. However, the use-fulness of such models, both for predictions and analyses, heavily depends on the placement and selection of rules (combined constituting the ML task of model selection). In this paper, we investigate a variety of techniques to efficiently place good rules within the search space based on their local prediction errors as well as their generality. This investigation is done within a specific LCS, named SupRB, where the placement of rules and the selection of good subsets of rules are strictly separated in contrast to other LCSs where these tasks sometimes blend. We compare a Random Search, $(1, \lambda)$ -ES and three Novelty Search variants. We find that there is a definitive need to guide the search based on some sensible criteria, i.e. error and generality, rather than just placing rules randomly and selecting better performing ones but also find that Novelty Search variants do not beat the easier to understand $(1, \lambda)$ -ES.

1 INTRODUCTION

With the ever increasing automation in many socio-technical settings, such as manufacturing, autonomous decisions of agents are more common than ever. This advent of more independent and intelligent technical systems holds great potentials in increasing safety and comfort of workers as well as general productivity. However, the roll-out of such systems can be held back when stakeholders, from operator to management level, do not trust that the systems perform on-par or even better than their human counterparts. Therefore, agents are required to give those stakeholders sensible explanations and insights into their decision making processes. (Heider et al., 2022a)

For the machine learning components of such agents, this means that they should offer strong interpretability, self-explaining or transparency-by-design capabilities. Recently, the use of Learning Classi-

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fier Systems (LCSs) (Urbanowicz and Moore, 2009) in such scenarios was proposed by (Heider et al., 2021). They argue that LCSs are uniquely suited as this family of rule-based learning algorithms features both powerful machine learning capabilities in all commonly encountered settings as well as inherently transparent models that follow human thought processes due to their rule-like structure. Rules in an LCS are of an if-then form, where the *if* (or condition) constricts the section of the feature space this rule applies to (matches) and the *then* contains a simpler, therefore more comprehensible, local model able to predict data points from that feature space partition. Conditions are usually optimized using a stochastic search heuristic, such as evolutionary algorithms. The model's practical transparency (or explainability in a broader context) is primarily influenced by the number of rules present and their placement within the feature space (the two tasks that constitute model selection in rule-based machine learning). Therefore, the-as optimal as possible-placement of rules should be a primary concern when designing an LCS algorithm with explainability requirements.

In this work, we expand the Supervised Rulebased learning system (SupRB) (Heider et al., 2022b),

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a recently proposed LCS for regression tasks, with different methods to discover new rules that fit the data well and benchmark them against each other on a variety of real world datasets.

2 LEARNING CLASSIFIER SYSTEMS AND RULE DISCOVERY

As previously introduced, LCSs are a family of typically evolutionary—rule-based learning systems with a long research history (Urbanowicz and Moore, 2009; Urbanowicz and Browne, 2017). Traditionally, they are categorized into two approaches:

- Michigan-style systems which feature strong online learning capabilities and have evolved from reinforcement learning (RL) to all major learning schemes. They consist of a single population of rules on which the optimizer operates directly.
- Pittsburgh-style systems that typically perform offline batch learning and primarily focus on supervised learning and feature a population of sets of rules, where the optimizer operates on those sets rather than the rules individually.

Due to those very different outsets, their approach to rule discovery and improvement differs substantially. For example, the most widespread Michiganstyle system, the XCS classifier system (Wilson, 1995), does feature two mechanisms to determine a new rule. The first is the covering mechanism. When the number of rules that match a new data point falls below a predetermined threshold, new rules are generated that match this data point. These rules are often randomly made more general than to just match this point specifically and therefore slightly differ when inserted into the population of rules. The second is the evolutionary algorithm. It is invoked on matching rules that also propose the chosen action (e.g. following an epsilon-greedy policy in RL). It utilizes crossover and mutation mechanisms appropriate for the types of input data and evolves the population in a steady-state manner.

For Pittsburgh-style systems, new rules can be directly added to an individual of the population (a set of rules), shared between individuals or be the product of a mutation (and more rarely rule-level crossover) operator. As the evolutionary algorithm of these systems operates on rule sets rather than rules directly, the fitness signal that guides evolution is not based on individual rule performance but rather the performance of a given set of rules, which can complicate rule discovery due to the added indirection.

3 THE SUPERVISED RULE-BASED LEARNING SYSTEM

The Supervised Rule-based learning system (SupRB) (Heider et al., 2022b) is an LCS with alternating phases of rule discovery and solution composition (additional details in (Heider et al., 2022c)). The two phases combined solve the standard machine learning task of model selection for an LCS. Splitting these phases allows a more direct control of the optimization process as objectives are more directly related to overall behaviour. In contrast, in Pittsburgh-style systems a model's fitness that also controls changes made to its rules follows the interaction of its rules rather than their individual suitability, whereas, in Michigan-style systems, rule fitness often depends on their neighbouring rules (niching) and, due to their online learning nature, does not necessarily relate to the full dataset. In the rule discovery (RD) phase of SupRB, new rules are generated and locally optimized to produce a diverse pool of general rules that exhibit low errors. Subsequently, in the solution composition (SC) phase, an optimizer attempts to select a well performing subset of the discovered rules. This subset should be small (exhibiting low complexity) but also produce a model (by mixing rules in areas of overlap) with a low prediction error. There is an obvious tradeoff between those two objectives (as was between general and accurate rules during RD). Thus, balancing these objectives highly depends on the use case at hand and the inherent requirements into explanations and model readability. In some cases, larger models might be acceptable, whereas, in others, e.g. when decisions need to be made fast, smaller models with less overlap are preferred.

The alternation between phases (rather than having a very long RD phase followed by an SC phase) allows to use additional information and guide the optimizers better. When discovering new rules, the RD mechanism places new rules more likely where the last elitist from the SC process showed high prediction errors. This can allow to fill unmatched areas (or areas of ill-fit local models) in the overall model that might otherwise go unnoticed. Blindly fitting a multitude of rules would become quite expensive as the whole dataset needs to be matched and then batchlearned multiple times. Additionally, it is hard to determine beforehand how many rules would be needed in the pool to find a satisfactory subset that solves the learning task.

SupRB's model is kept as simple and interpretable as possible as its transparency is a central aspect (Heider et al., 2022b):

- 1. Rules' conditions use an interval based matching: A rule *k* applies for example *x* iff $x_i \in [l_{k,i}, u_{k,i}] \forall i$ with *l* being the lower and *u* the upper bounds.
- 2. Rules' local models $f_k(x)$ are linear. They are fit using linear least squares with a l2-norm regularization (Ridge Regression) on the subsample matched by the respective rule.
- 3. When mixing multiple rules to make a prediction, a rule's experience (the number of examples matched during training and therefore included in fitting the submodel) and in-sample error are used in a weighted sum.

For the SC phase optimizer, we use a genetic algorithm (GA) for all experiments in this paper. It operates directly on a bitmap corresponding to whether a rule from the pool is part of this solution to the learning task at hand or whether it is not. In previous work by (Wurth et al., 2022) other metaheuristic optimizers were tested to compose solutions. They found that the choice of metaheuristic is-given sufficient computational budget-largely dependent on the learning task, although even there, differences were small, which makes the GA a fitting choice. This is also the more traditional option as LCSs typically feature evolutionary computation methods. Parent (groups of two) selection is done using tournament selection. Those parents are recombined with an *n*-point crossover under a 90% probability. The children are then mutated using a probabilistic bit-flip mutation. These children form the new population together with the fittest parents (elitism). In our experiments we used a population size of 32 children and 5 to 6 elitists. An individual's (solution to the learning task) fitness is determined based on its insample prediction error and its complexity (number of rules present) following (Heider et al., 2022b). Critically, this phase does not affect the position of rules' bounds. Individuals can only be composed of rules in the pool and those rules remain unchanged by the GA's operators.

The main subject of this paper is the RD phase's optimizer. In contrast to many typical optimization problems we do not want to find the singular globally optimal rule but rather a set of localized rules that perform well in this particular feature space partition, thus, we are attempting to find an unknown number of local optima without mapping the entire fitness landscape. The rules discovered should be a diverse set and we can allow overlapping rules as SC will select the subset of discovered rules most appropriate to solve the learning task. As for the SC, a variety of different optimizers can achieve this. In the following, the five different optimization approaches for RD that will be compared in the remainder of this paper

are presented. For all heuristics we utilize the same approach for calculating rule fitness by combination of two objectives, utilizing the in-sample error and the matched feature space volume, respectively—cf. (Heider et al., 2022b).

3.1 Evolution Strategy

As discussed before, LCSs traditionally apply some evolutionary algorithm for their optimization processes. Therefore, the first strategy employed for RD in SupRB, which was also used for the experiments in (Wurth et al., 2022), is an *Evolution Strategy* (ES) (Heider et al., 2022b), specifically, a simplified $(1, \lambda)$ -ES. The initial individual for the ES is generated by placing a rule at a randomly selected training example, preferring those examples where the in-sample error is high in the intermediate global solution. This individual serves as the initial candidate for addition to the pool and the parent. From the parent, λ children are generated, each mutated by a non-adaptive operator which moves the upper and lower bounds further outwards by adding values sampled from a halfnormal distribution. The parent for the next generation is the child individual with the highest fitness. If this individual showed a better fitness than the current candidate it also becomes the new candidate. The evolutionary search terminates when for a fixed number of generations no new candidate has been found. This ES produces one rule at a time but can easily be parallelized. One merit of this approach is in the explainability of both the search procedure and the resulting pool. In general, rules that have fitnesses independent from other rules are easier to understand for most non-experts. Whereas, in most current LCSs, the fitness assigned to a rule is highly dependent on what other rules it is surrounded by. Beyond fitnessbased considerations on the understandability of our approach, the ES is also a quite easy to follow search method: Expand the area (or hypervolume) an individual matches, evaluate the new individuals, choose the best new option and repeat.

3.2 Random Search

As an alternative to the strongly fitness-guided RD performed by the ES, *Random Search* (RS) is introduced. RS commonly serves as a baseline for testing the performance of other optimization algorithms. Furthermore, with the ulterior motive of finding diverse rules to add to the pool, RS provides an interesting approach where the fitness only plays a role in the selection of the final candidate, but not in the generation of new rules. In SupRB, RS, similarly to ES, randomly selects a fixed number of data points weighted by their respective in-sample prediction errors in the last solution candidate (produced by the previous SC phase). We then place random bounds around those points based on half-normal distributions (to ensure we always match the selected point). To balance the computational cost between RD approaches, we produce substantially more rules initially than we would in an ES generation. We then greedily select the rule with the highest fitness to become part of the pool.

3.3 Novelty Search

One of the central issues of RD is that the optimizer is tasked to find multiple rules that partition the feature space and, in their individual area, predict data points well, whereas in many typical optimization problems the optimizer would be expected to find a single global optimum (or at least a point very close to it). This task the optimizer has to complete can somewhat be viewed as being tasked to map the larger local optima within the search space. We aim at finding a diverse set of good rules, each within their specific area.

In this section, we describe an approach based on Lehman's Novelty Search (NS) (Lehman, 2012). In this evolutionary search method the optimizer is not (or not fully) guided by the typical fitness function but rather tries to find individuals that exhibit new behaviour previously unknown within the population. Mapped to our case, where we want to find a rule that predicts an area of the feature space currently unmatched or only matched by rules with high errors in this area, behaviour of rules can be equated to what subsample of the training data they match. For our adaptation, we base the NS on a (μ, λ) -ES with elitism and follow the extensive experimental findings laid out by (Gomes et al., 2015). In each iteration, we select a list of λ parents out of the current population. These parents are paired, undergo a uniform crossover and a half-normal mutation (cf. Section 3.1). The resulting children are then fitted and the best performing μ children are selected for the next population. Additionally, we select a number of high-performing parents equal to the number of rules the NS is expected to produce within one RD phase as part of the new population (elitism). Performance of an individual can be based on novelty alone or on a combination of fitness (as used in the ES; cf. Section 3.1) and novelty, e.g. a linear combination. For the novelty of a rule, we compare its match set and the match sets of the other rules in the pool and the current NS population (the other children for the selection or the parents for elitism,

respectively). The novelty score assigned to a rule is the average Hamming-distance between its match set and its k nearest neighbours' (most similar rules). k is set to 15; a value typically encountered with other NS applications in literature—e.g. (Lehman and Stanley, 2010). After a set number of iterations, we add a set number of rules to the pool and conclude this phase. Which rules get added can be randomized or based on the highest novelty(-fitness combination).

In addition to the basic NS, we implemented and experimented with two variants: *Minimal Criteria Novelty Search* (MCNS) (Lehman and Stanley, 2010; Lehman, 2012) and *Novelty Search with Local Competition* (NSLC) (Lehman, 2012).

MCNS imposes additional pressure on the search to explore less vividly and focus more on rules that at least fulfil some minimal requirement. In our experiments, we set the minimal criterion to a minimum number (tuned between 10 and 20) of examples from the training data having to be matched by the rule to become viable. Although, we did also impose that at most one fourth of the population should be removed because they missed the minimal criterion to prevent collapsing gene pools. We also use progressive minimal criteria novelty search (Gomes et al., 2012), itself based on MCNS, as an option for combining fitness and novelty as the objective. Here, all individuals that do exhibit a fitness worse than the median fitness are removed automatically in each iteration of the search. This approach is not tied to MCNS and can be used in all three variants.

NSLC introduces a localised fitness-based pressure on the new generation. The idea is that, within a neighbourhood (based on their behaviour and not their position in the search space) of similar rules, the rules that exhibit high fitnesses should be chosen. A rule's novelty score gets increased by a factor of b/κ , where *b* is the number of individuals within the neighbourhood specified by κ that have a worse fitness than the rule currently evaluated. We chose κ to be equal to *k* as this already does specify a neighbourhood of rules this rule is in competition with.

One disadvantage of NS-like approaches is that rule selection is no longer solely based on independent metrics (fitness) but rather on the independent fitness and the highly dependent (on other rules) novelty score.

4 EVALUATION

To examine the differences between the rule discovery methods and to find the most versatile strategy, we evaluated those strategies within SupRB on several regression datasets.

4.1 Experiment Design

SupRB is implemented¹ in Python 3.9, adhering to scikit-learn (Pedregosa et al., 2011) conventions. Input features are transformed into the range [-1, 1], while the target is standardized. Both transformations are reversible but improve SupRB's training process as they help preventing rules to be placed in regions where no sample could be matched and remove the need to tune error coefficients in fitness calculations, respectively. Based on our assumptions about the number of rules needed, 32 cycles of alternating rule discovery and solution composition are performed, generating four (or 8 in case of NS variants) rules in each cycle for a total of 128 (256 for NS variants) rules. Additionally, the GA is configured to perform 32 iterations with a population size of 32. To tune some of the more sensitive parameters, we performed a hyperparameter search using a Tree-structured Parzen Estimator in the Optuna framework (Akiba et al., 2019) that optimizes average solution fitness on 4-fold cross validation. We tuned the optimizers on each dataset independently for a fixed tuning budget of 360 core hours. The final evaluation, for which we report results in Section 4.2, uses 8-split Monte Carlo cross-validation, each with 25% of samples reserved as a validation set. Each learning algorithm is evaluated with 8 different random seeds for each 8-split cross-validation, resulting in a total of 64 runs.

Table 1: Overview of the regression datasets the five rule discovery approaches for SupRB are compared on.

Name	n _{dim}	n _{sample}
Combined Cycle Power Plant	4	9568
Airfoil Self-Noise	5	1503
Concrete Strength	8	1030
Energy Efficiency Cooling	8	768

We evaluate on four datasets part of the UCI Machine Learning Repository (Dua and Graff, 2017). An overview of sample size and dimensionality is given in Table 1. The Combined Cycle Power Plant (CCPP) (Kaya and Tüfekci, 2012; Tüfekci, 2014) dataset shows an almost linear relation between features and targets and can be acceptably accurately predicted using a single rule. Airfoil Self-Noise (ASN) (Brooks et al., 1989) and Concrete Strength (CS) (Yeh, 1998) are both highly non-linear and will likely need more rules to predict the target sufficiently. The CS dataset has more input features than ASN but is easier to predict overall. Energy Efficiency Cooling (EEC) (Tsanas and Xifara, 2012) is another rather linear dataset, but has a much higher input features to samples ratio compared to CCPP. It should similarly be possible to model it using only few rules.

4.2 Results

In the following we abbreviate *SupRB using X as RD method* simply by *X*.

The means and standard deviations of model performances (measured using the—standardized individually per dataset—*mean squared error* on test data (MSE)) and model complexities (measured by the number of rules in the final elitist) achieved by the five RD approaches when evaluated—as described in the previous section—on the four real-world datasets are given in Tables 2 and 3. At first glance, on all four datasets, RS shows the worst performance in terms of mean MSE and, with the exception of CS, the models it creates also have the highest model complexity. The other four optimization approaches vary in their results between datasets.

In order to get a better overview as well as include distributional information, we create violin plots to visualize the MSE results (Figure 1). It can be seen that, on CCPP (top left in Figure 1), the distributions of MSE values achieved look very similar, with NS and NSLC maybe having a very slight edge (consider the y axis scale) which is not visible in the rounded mean and standard deviations given in Table 2. For the ASN dataset, the corresponding violin plot (top right in Figure 1) as well as the values in Table 2 suggest that ES outperforms the other optimizers and NSLC is slightly better than NS and MCNS. However, with respect to model complexity (Table 3), we observe inverse results: NS and MCNS depict a similarly low model complexity, while the mean number of rules in the solutions found by NSLC, ES and RS is higher by more than ten. When regarding the CS dataset, Table 2 and Figure 1 (bottom left) hint towards NSLC being the best of the considered methods with ES, NS and NSLC performing similarly to each other but slightly worse than NSLC. In terms of model complexity (Table 3), this is, again, reversed: ES, NS and MCNS are similar once more and result in less complex solutions than NSLC. For the last dataset, EEC, ES is indicated again as the best performing method (bottom right in Figure 1). The

¹Recent code at: https://github.com/heidmic/suprb. The specific version of the code used in this paper can be found at: https://doi.org/10.5281/zenodo.7059913.

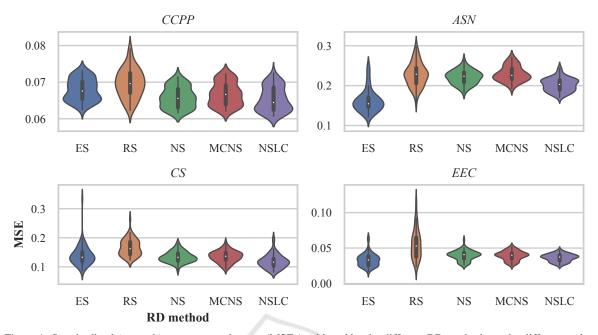


Figure 1: Standardized (per task) mean squared errors (MSEs) achieved by the different RD methods on the different tasks.

Table 2: Mean and standard deviation (over 64 runs, rounded to two decimal places) of MSE achieved by the five RD approaches on the four datasets. Best entry in each row (if one exists) marked in bold.

CCPP 0.07 ± 0.00 ASN 0.16 ± 0.03 0.23 ± 0.03 0.22 ± 0.02 0.23 ± 0.02 0.20 ± 0.02 CS 0.14 ± 0.04 0.17 ± 0.03 0.13 ± 0.02 0.13 ± 0.02 0.12 ± 0.02		ES	RS	NS	MCNS	NSLC
	CCPP	0.07 ± 0.00	0.07 ± 0.00	0.07 ± 0.00	0.07 ± 0.00	0.07 ± 0.00
CS 0.14 ± 0.04 0.17 ± 0.03 0.13 ± 0.02 0.13 ± 0.02 0.12 ± 0.02	ASN	0.16 ± 0.03	0.23 ± 0.03	0.22 ± 0.02	0.23 ± 0.02	0.20 ± 0.02
	CS	0.14 ± 0.04	0.17 ± 0.03	0.13 ± 0.02	0.13 ± 0.02	0.12 ± 0.02
EEC 0.03 ± 0.01 0.06 ± 0.02 0.04 ± 0.01 0.04 ± 0.01 0.04 ± 0.01	EEC	0.03 ± 0.01	0.06 ± 0.02	0.04 ± 0.01	0.04 ± 0.01	0.04 ± 0.01

model complexity, however, is lower for NSLC and much lower for NS and MCNS.

Overall, the visual analysis combined with the rounded statistics of mean and standard deviation are not capable of providing us with a conclusive answer regarding which of the RD methods should be preferred on tasks like the ones considered. We thus investigate the data gathered more closely using Bayesian data analysis².

We start by applying to our data the model proposed by Calvo et al. (Calvo et al., 2018; Calvo et al., 2019) which, for each of the RD methods, provides us with the *posterior distribution over the probability of that RD method performing best*. We apply this model to both the MSE observations as well as the model complexity observations and provide box plots (Figures 2 and 3) which show the most relevant distribution statistics. Both figures show that the distributions over the probabilities of performing the best are rather tight. However, the figures also show that there cannot be made a very confident conclusive statement for a single RD method given the data available: For both metrics, the highest expected value for the probability of being the best assigned by the model to a single RD method is only around 40 % (to illustrate: this means that the probability of that candidate not being the best is around 60 %). Due to this, we also considered the probability distribution over the probability of either ES or NSLC performing the best MSE-wise since those were the highest probability candidates with respect to that metric. As can be seen, for MSE, the probability of either of the two being ranked the best is still merely around 60 % which still does not amount to much evidence. Only if we include the top three options (ES, NSLC and NS), are we entering the region of over 80% where we could say with some slight confidence that the best-performing is among those three.

When considering model complexity (Figure 3), there is an 80 % probability that one of NS and MCNS performs the best. However, since the probability of each of these not performing the best MSE-wise is around 80 % or more, we do not consider them to be

²We deliberately do not use null hypothesis significance tests due to their many flaws and possible pitfalls—cf. e.g. (Benavoli et al., 2017).

		ES	RS	NS	MCNS	NSLC	
	CCPP	04.52 ± 1.48	12.86 ± 3.13	05.84 ± 0.91	06.02 ± 1.39	06.94 ± 1.41	
	ASN	31.78 ± 2.21	32.98 ± 3.11	18.22 ± 2.91	18.81 ± 2.46	29.75 ± 3.84	
	CS	24.95 ± 2.45	29.56 ± 2.47	23.50 ± 3.47	22.38 ± 3.02	33.83 ± 3.28	
	EEC	12.94 ± 2.10	30.17 ± 3.78	06.92 ± 1.70	06.22 ± 1.13	10.16 ± 1.94	
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Table 3: Mean and standard deviation like Table 2 but for model complexity.

Figure 2: Box plot (with standard 1.5 IQR whiskers and outliers) of the posterior distribution obtained from the model by Calvo et al., 2018; Calvo et al., 2019) applied to the MSE data. An RD method having a probability value of q% says that the probability of that RD method performing the best with respect to MSE is q%. In addition to each individual RD method we also included the distributions for "either of ES or NSLC (or NS) perform best".

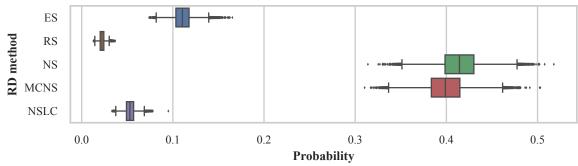
competitive enough to merit a closer analysis within the present work.

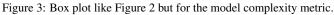
We next consider the difference in performance between ES (since it is both the originally-used RD method as well as the runner-up with respect to the probability of being the best MSE-wise) and NSLC (since it has the highest probability of having the lowest MSE) by applying Corani and Benavoli's Bayesian correlated t-test (Corani and Benavoli, 2015). The resulting posteriors (given in Figures 4 and 5 including 99 % HDIs) are the distribution of the difference between the considered metric for NSLC and the considered metric for ES (which means that values larger than zero indicate NSLC having a higher (worse) metric value than ES). It can be seen that, on the CCPP dataset, the difference in MSEs between NSLC and ES is most certainly negligible in practice which corroborates the earlier statement that on that dataset all but RS perform similarly. On ASN, on the other hand, ES outperforms NSLC by an MSE of at least 0.04 with a probability of over 99 $\%^3$ (99 %of probability mass already lies between the dashed lines alone and even more to the right the upper HDI bound). The probability of NSLC outperforming ES

on the CS dataset by an MSE of 0.019 to 0.022 is 99%. On EEC, the last of the four datasets, there is, again, not really a significant difference to be noticed (e.g. if a difference in MSE of 0.0033 could be considered not practically relevant on this dataset then the two should be considered to perform equivalently with a probability of over 99%).

Things look differently when regarding the model complexities produced by the two approaches (Figure 5). On each of the datasets, there is considerable probability mass on each side of 0. While we could simply compute the integral to the left (or right) of 0, this would include differences that are not relevant in practice. We thus decided to define a region of practical equivalence (rope) centered on a complexity difference of 0. Since the learning tasks are very different in their model complexity (i.e. require different solution sizes), we opted for a task-dependent rope. As this is difficult to choose based on the task alone (i.e. requiring detailed domain knowledge about the different processes that generated the data), we let the collected data inform our choice of the rope for each task: We choose as the bounds of the rope the mean of the standard deviations of ES, NS, MCNS and NSLC (leaving out RS since that method does not even remotely achieve competitive results with respect to solution complexity). The rope for each task is included

 $^{^{3}}$ This means that in over 99 % of future runs we would expect the MSE difference between the two approaches to be at least 0.04.





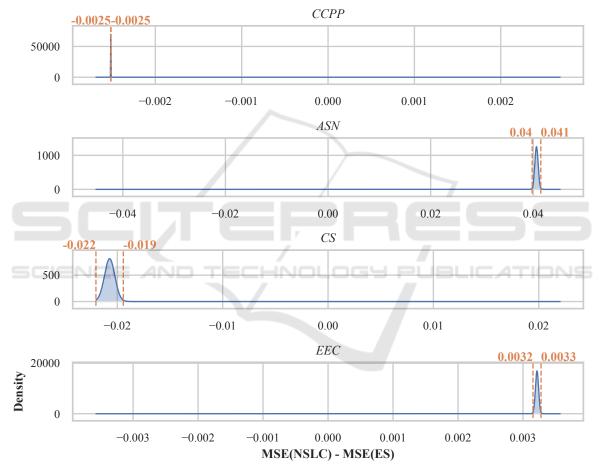


Figure 4: Density plot of the posterior distribution obtained from Corani and Benavoli's Bayesian correlated t-test (Corani and Benavoli, 2015) applied to the difference in MSE between NSLC and ES. Orange dashed lines and numbers indicate the 99 % HDI (i.e. 99 % of probability mass lies within these bounds). HDI bounds rounded to two significant figures.

in Figure 5 as a green area delimited by green dotted lines. Based on the rope and the Bayesian correlated t-test model we can now compute the probabilities for ES and NSLC performing practically equivalently or worse than the other; they are given in Table 4. Upon close inspection we can determine that for ASN, the data is not conclusive. For CCPP and CS, ES produces less complex solutions than NSLC with a probability of 75.1 % and 86.2 % respectively. For EEC there is *some* evidence hinting towards NSLC creating more compact solutions, however, this, again is not fully conclusive as the probability of this not being the case is 34.4 %.

We conclude our analysis with a summary of the key takeaways.

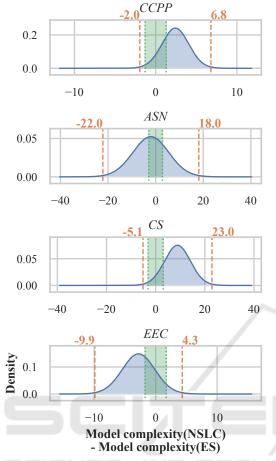


Figure 5: Density plot like Figure 4 but for the model complexity metric and with the region of practical equivalence (rope) marked by green dotted lines and a green area.

Table 4: Probability (in percent, rounded to one decimal place) of ES or NSLC performing better or worse than the other—or practically equivalently—with respect to model complexity.

	ES worse	pract. equiv.	NSLC worse
CCPP	1.3	23.5	75.1
ASN	45.6	28.4	26.0
CS	1.4	12.4	86.2
EEC	65.6	29.6	4.9

- NSLC has the highest probability of being the best option MSE-wise on datasets like the ones we considered. However, the data we collected is not entirely conclusive with respect to that (there is still an around 60 % chance of NSLC *not* having the best MSE on such datasets).
- When considering model complexity alone, there is a high probability of either of NS or MCNS being the best—however, their MSEs are with a high probability not the best.

- A closer comparison of ES with NSLC yielded:
 - ES outperforms NSLC MSE-wise with very high probability (> 99%) by a presumably practically relevant amount on ASN whereas this is the other way around on CS. However, on these two tasks, the data is either not conclusive as to which method yields the better model complexities (ASN) or the method with the worse MSE performs better in that regard (CS).
 - On the other two tasks, ES and NSLC perform somewhat equivalently MSE-wise. There is some light evidence for ES yielding better model complexities on the less difficult of these (CCPP) and for NSLC yielding better model complexities on the more difficult one (EEC).
- Overall, we can say that despite its simplicity when compared to the other approaches, the (1,λ)-ES performs not worse when only considering *practically relevant differences*.

5 CONCLUSION

This work investigated the use of different evolutionary approaches towards rule discovery in the Supervised Rule-based learning system (SupRB), a recently proposed Learning Classifier System (LCS) for regression problems. This system's key characteristic is the separation of finding a diverse pool of rules that fit the data well from their composition into a model that is both accurate and uses a minimal number of rules—a key advantage when employed in settings where model transparency is important, such as typical explainable artificial intelligence applications. By determining from intermediate solutions which areas of the problem space were already well covered, subsequent evolution can be guided towards other areas to form new rules there and, therefore, improve the overall diversity of the available rules.

The investigated methods were a $(1, \lambda)$ -ES, a Random Search (RS) and three Novelty Search (NS) variants. The NS-based variants all employed a (μ, λ) -ES, scored a rule's novelty on the basis of its match set and combined it with traditional fitness. Besides a traditional NS, we investigated Minimal Criteria Novelty Search (MCNS) and Novelty Search with Local Competition (NSLC).

After an evaluation of the five methods on four real-world regression problems, we found that performances are similar but, depending on the dataset, specific methods can be preferred, with ES and NSLC being the most interesting candidates. This was confirmed by a rigorous statistical analysis. Interestingly, we found that where ES can be expected to perform better on error than NSLC, it can also be expected to yield larger solution sizes (a higher number of rules in the model) and vice versa.

Overall, we recommend to use either ES or NSLC, although, due to its greater simplicity and the fact that rules are selected independently of the status of other rules, ES seems to be the preferential candidate for cases where model construction is important for the explainability requirements of users.

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REFERENCES

- Akiba, T., Sano, S., Yanase, T., Ohta, T., and Koyama, M. (2019). Optuna: A Next-generation Hyperparameter Optimization Framework. In *Proceedings* of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, KDD '19, pages 2623–2631, New York, NY, USA. Association for Computing Machinery.
- Benavoli, A., Corani, G., Demšar, J., and Zaffalon, M. (2017). Time for a change: A tutorial for comparing multiple classifiers through bayesian analysis. J. Mach. Learn. Res., 18(1):2653–2688.
- Brooks, T., Pope, D., and Marcolini, M. (1989). Airfoil Self-Noise and Prediction. Technical Report RP-1218, NASA.
- Calvo, B., Ceberio, J., and Lozano, J. A. (2018). Bayesian inference for algorithm ranking analysis. In Proceedings of the Genetic and Evolutionary Computation Conference Companion, GECCO '18, pages 324–325, New York, NY, USA. Association for Computing Machinery.
- Calvo, B., Shir, O. M., Ceberio, J., Doerr, C., Wang, H., Bäck, T., and Lozano, J. A. (2019). Bayesian performance analysis for black-box optimization benchmarking. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, GECCO '19, pages 1789–1797, New York, NY, USA. Association for Computing Machinery.
- Corani, G. and Benavoli, A. (2015). A bayesian approach for comparing cross-validated algorithms on multiple data sets. *Machine Learning*, 100(2):285–304.
- Dua, D. and Graff, C. (2017). UCI machine learning repository. http://archive.ics.uci.edu/ml.
- Gomes, J., Mariano, P., and Christensen, A. L. (2015). Devising effective novelty search algorithms: A comprehensive empirical study. In *Proceedings of the*

2015 Annual Conference on Genetic and Evolutionary Computation, GECCO '15, page 943–950, New York, NY, USA. Association for Computing Machinery.

- Gomes, J., Urbano, P., and Christensen, A. L. (2012). Progressive minimal criteria novelty search. In Pavón, J., Duque-Méndez, N. D., and Fuentes-Fernández, R., editors, Advances in Artificial Intelligence – IB-ERAMIA 2012, pages 281–290. Springer Berlin Heidelberg.
- Heider, M., Nordsieck, R., and Hähner, J. (2021). Learning Classifier Systems for Self-Explaining Socio-Technical-Systems. In Stein, A., Tomforde, S., Botev, J., and Lewis, P., editors, *Proceedings of LIFELIKE* 2021 co-located with 2021 Conference on Artificial Life (ALIFE 2021).
- Heider, M., Stegherr, H., Nordsieck, R., and Hähner, J. (2022a). Learning classifier systems for selfexplaining socio-technical-systems. https://arxiv.org/ abs/2207.02300. Submitted as an extended version of (Heider et al., 2021).
- Heider, M., Stegherr, H., Wurth, J., Sraj, R., and Hähner, J. (2022b). Separating Rule Discovery and Global Solution Composition in a Learning Classifier System. In Genetic and Evolutionary Computation Conference Companion (GECCO '22 Companion).
- Heider, M., Stegherr, H., Wurth, J., Sraj, R., and Hähner, J. (2022c). Investigating the impact of independent rule fitnesses in a learning classifier system. http://arxiv. org/abs/2207.05582. Accepted for publication in the Proceedings of BIOMA'22.
- Kaya, H. and Tüfekci, P. (2012). Local and Global Learning Methods for Predicting Power of a Combined Gas
 & Steam Turbine. In Proceedings of the International Conference on Emerging Trends in Computer and Electronics Engineering ICETCEE.
- Lehman, J. (2012). *Evolution Through the Search for Novelty*. PhD thesis, University of Central Florida.
- Lehman, J. and Stanley, K. O. (2010). Revising the evolutionary computation abstraction: Minimal criteria novelty search. In *Proceedings of the 12th Annual Conference on Genetic and Evolutionary Computation*, GECCO '10, page 103–110, New York, NY, USA. Association for Computing Machinery.
- Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, É. (2011). Scikit-learn: Machine Learning in Python. *The Journal of Machine Learning Research*, 12:2825–2830.
- Tsanas, A. and Xifara, A. (2012). Accurate Quantitative Estimation of Energy Performance of Residential Buildings Using Statistical Machine Learning Tools. *Energy and Buildings*, 49:560–567.
- Tüfekci, P. (2014). Prediction of full load electrical power output of a base load operated combined cycle power plant using machine learning methods. *International Journal of Electrical Power & Energy Systems*, 60:126–140.

- Urbanowicz, R. J. and Browne, W. N. (2017). *Introduction* to Learning Classifier Systems. Springer Publishing Company, Incorporated, 1st edition.
- Urbanowicz, R. J. and Moore, J. H. (2009). Learning Classifier Systems: A Complete Introduction, Review, and Roadmap. *Journal of Artificial Evolution and Applications*.
- Wilson, S. W. (1995). Classifier fitness based on accuracy. Evolutionary Computation, 3(2):149–175.
- Wurth, J., Heider, M., Stegherr, H., Sraj, R., and Hähner, J. (2022). Comparing different metaheuristics for model selection in a supervised learning classifier system. In *Genetic and Evolutionary Computation Conference Companion (GECCO '22 Companion).*
- Yeh, I.-C. (1998). Modeling of Strength of High-Performance Concrete Using Artificial Neural Networks. *Cement and Concrete Research*, 28(12):1797– 1808.

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