AMS: Generating AutoML search spaces from weak specifications

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ABSTRACT

We consider a usage model for automated machine learning (AutoML) where users can influence the output pipeline by providing a *weak pipeline specification.* A weak specification is an unordered set of API components, which the AutoML tool can include in its output pipeline. This specification allows users to express preferences over the resulting components, such as the desire for interpretability. We present AMS, an approach to automatically strengthen such a specification to include unspecified complementary and functionally related API components, populate the space of hyperparameters and their values, and pair this configuration with a search procedure to produce a *strong pipeline specification*: a full description of the search space for candidate pipelines. AMS uses normalized pointwise mutual information on a code corpus to identify complementary components, BM25 as a lexical similarity score over the target API's documentation to identify functionally related components, and frequency distributions in the code corpus to extract key hyperparameters and values. We show that strengthened specifications can produce pipelines that outperform the initial specification and an expert-annotated variant, while producing pipelines that reflect the bias of the original specification.

1 INTRODUCTION

Automated Machine Learning (AutoML) [15, 23, 26, 36] promises to democratize the use of machine learning techniques by end-users, allowing non-experts access to a tool that has become standard for tackling research and applications across domains as diverse as medicine, finance, and software engineering [17, 28, 33, 35]. AutoML tools typically take as input a tabular dataset along with a classification or regression task (i.e. predict a particular column) and generate an optimized composition of machine learning operators, drawn from a target API, to produce an executable pipeline.

At the core of AutoML tools lie search procedures that generate and evaluate possible pipeline candidates. Under the prevailing usage model [45], the end-user treats the AutoML tool as a black-box which returns a pipeline that outperforms other candidates generated based on some predictive performance metric (e.g. F1 score). In this setting the end-user has no direct way of influencing the pipeline chosen by the system. However, a user may need to express preferences, beyond maximizing a predictive performance metric, to satisfy constraints such as pipeline interpretability, domain-specific best practices, and data scaling constraints, for example.

We propose the use of a *weak pipeline specification* as a way to provide partial user preferences to the AutoML tool. A weak pipeline specification consists of an unordered set of API components that the end-user may want in their resulting pipeline. This specification can be automatically extended to produce a *strong pipeline specification* that captures additional API components of interest, defines a set of hyperparameters and values to search over, and a search procedure to sample candidate pipelines. The strengthened pipeline specification can then influence the output pipeline produced by the AutoML tool by constraining the search space.

For example, the user might provide { logistic regression } as a weak specification. Strengthening this specification could add other linear models (e.g. linear SVM), would specify different possible types of regularization (e.g. L1/L2) and their weights, and would include the search procedure (e.g. genetic programming) used to sample pipelines. This proposed model of interaction allows the end-user greater control over the eventual output pipeline, without negating the key advantage of AutoML: the user need not be an ML expert.

We introduce a novel system, AMS (Figure 1), that automatically strengthens AutoML search space specifications. To carry out this strengthening, AMS exploits information in a code corpus and the target API's documentation. First, AMS automatically mines pairs of complementary API components from the selected code corpus, where two components are complementary if they co-occur frequently. To formalize this mining procedure, AMS uses normalized pointwise mutual information [5] to rigorously characterize co-occurrence in probabilistic terms. These mined associations can then be used to extend the initial weak specification. Next, AMS identifies unspecified API components that may be functionally related to those in the original specification. To reason about component similarity, AMS applies BM25 [41], a popular and effective measure of lexical similarity, over the API's documentation. With this metric, AMS can identify components with the highest degree of relation to those in the original specification. Next, given that machine learning pipelines are known to exhibit different performance based on hyperparameter values [39], AMS uses frequency distributions, estimated from the selected code corpus, to define a hyperparameter search space for each component in the extended specification. Finally, AMS pairs this component configuration with a search procedure, which is used to sample candidate pipeline from the given space.

We empirically evaluate AMS's predictive performance, in terms of macro-averaged F1 score, over 9 datasets and 15 weak pipeline specifications. Our results show that, with two different search procedures, AMS can produce pipelines that outperform the pipelines obtained using the initial weak specification and an expert-annotated version of the weak specification including hyperparameters and values. To quantify the extent of outperformance, we use the concept of a *win*. A pipeline wins when it obtains the highest score on a specification/dataset combination, and satisfies a minimum predictive score difference to rule out comparable scores.

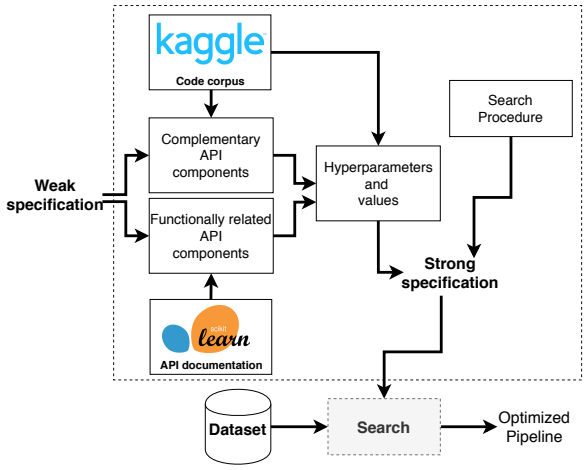


Figure 1: AMS system diagram. System boundaries are depicted as a dashed line. The user provides a weak specification. This specification is automatically extended to include complementary and functionally related API components. For each component, AMS identifies key hyperparameters and possible values. This configuration is paired with a search procedure to produce a strong specification, which can be used to search for pipelines targeting a user-provided dataset.

When using genetic programming as a search procedure, AMS's specifications result in 38 wins compared to 12 under the weak specification extended with an expert hyperparameter space. When using random search as a search procedure, AMS's specifications result in 41 wins compared to 14 wins under the weak specification extended with an expert hyperparameter space. We also find that the pipelines produced using AMS's specification qualitatively reflect the influence of the weak specification.

To summarize, this paper makes the following contributions:

- We present a novel approach to automatically strengthen pipeline specifications for AutoML tools, allowing users to influence the final pipeline produced. Our approach relies on a probabilistic characterization of co-occurring API components, lexical similarity over alternative components' API documentation, and frequency distributions for hyperparameter spaces.
- We implement this approach (and share our evaluation dataset) in an open-source system called AMS[1].
- We evaluate AMS using 9 datasets from an existing AutoML paper [36], 15 weak pipeline specifications, and two different search procedures. Our results show that AMS's strengthened specifications produce higher performing pipelines. When using genetic programming, AMS specifications produced 38 wins compared to 12 from an expert-annotated variant of the weak specification, and 9 from the original weak specification. We see a similar number of wins when comparing approaches using random search.
- We qualitatively show that the distribution of components in the output pipelines produced using AMS specifications reflect the influence of the initial weak specification.

In the following sections we review the background on AutoML (Section 2), introduce the notion of pipeline specifications (Section 3), provide an illustrative scenario for the use of AMS (Section 4), detail the approach and design of AMS (Section 5), present experimental results (Section 6), provide context on related work (Section 7), outline possible threats (Section 8) and conclude (Section 9).

2 AUTOML BACKGROUND

We first formally introduce AutoML for classification [26]. Let $d \in \mathcal{D} : \mathbb{R}^{n \times m} \times \mathbb{N}^n$ be a dataset comprised of a matrix of n observations, each with m real covariates, and a vector of n natural number labels. Let $\mathcal{H} : \mathbb{R}^{n \times m} \rightarrow \mathbb{N}^n$ be the type of a pipeline program defined as a composition of preprocessing and learning algorithms – implemented as API components in a target library – along with their corresponding hyperparameter settings. A pipeline takes a dataset and predicts labels based on covariates. Let $\mathcal{S}$ be the search space of all possible pipeline programs. Let $e \in \mathcal{E} : \mathcal{H} \times \mathcal{D} \rightarrow \mathbb{R}$ be an evaluation function that scores the ability of a pipeline to successfully predict labels and generalize to unseen observations (e.g. cross-validated F1 score). Let $\text{cost} \in C : \mathcal{H} \times \mathcal{D} \rightarrow \mathbb{R}$ be a cost function that evaluates pipeline execution time on a dataset d, and $b \in \mathbb{R}$ be a search time budget. Then AutoML corresponds to the optimization problem

$$\underset{h \in \mathcal{S}}{\text{argmax}}\, e(h,d) \; s.t. \sum_{h \in \mathcal{S}} \text{cost}(h,d) \leq b$$

Given that the possible space of pipelines $\mathcal{S}$ is exponentially large, it is impractical to evaluate every pipeline in $\mathcal{S}$ within the given budget b. Effective AutoML systems will therefore typically have to perform a search over the space, evaluating only a subset of pipelines. The AutoML system iteratively searches and evaluates pipelines in $\mathcal{S}$, keeping track of its estimate of the best pipeline.

2.1 Searching the Pipeline Space

Existing AutoML systems employ a variety of search strategies to identify candidate pipelines. These strategies include genetic programming [36], Bayesian optimization [15], reinforcement learning [11], program-analysis-based search [7], and random search [18].

To improve the effectiveness of these strategies, systems may also incorporate prior-knowledge about pipeline performance or impose additional structure on the candidate pipelines that can be generated. For example, an AutoML system may warm-start the search by incorporating previously successful pipelines [15, 44], condition on textual dataset and algorithm descriptions [12], manually constrain the subset of algorithms available for pipeline definitions [36], or constrain the shape of possible pipelines [10, 11]. The latter two provide ways to restrict the type of pipelines produced, however, they require user involvement and expertise. In the following section, we present an approach that bridges this gap.

3 PIPELINE SPECIFICATIONS

The current usage model for AutoML typically emphasizes the lack of user involvement [45]. Under this model, the user presents the tool

[1] https://anonymous.4open.science/r/27365419-337b-4a64-be3f-0cd17d830c58/

with their target dataset, for which they want to learn a classification pipeline, sets some computational budget, runs the tool, and accepts the pipeline produced by the AutoML tool. In this context, the AutoML tool receives no user feedback (beyond the input dataset), and the user is unable to influence the pipelines considered by the search procedure. Without any formal user feedback, the AutoML tool is unable to 1) exploit any user domain knowledge or 2) provide a pipeline that satisfies any desired user constraints (e.g. interpretability).

We propose the use of *weak specifications* as a way for AutoML users to automatically influence the pipelines produced by constraining the search space for candidates generated by the AutoML tool.

Definition 3.1. Weak Specification. A weak specification is an (unordered) set of API components.

By providing a set of API components a user provides (partial) information regarding what they want: specifically a set of algorithms (e.g. classifiers, preprocessors) that should be considered for pipeline generation. We call this type of specification *weak* as it is incomplete along four key dimensions:

(1) it does not specify what hyperparameters are relevant
(2) it does not specify what values hyperparameters can take on
(3) other relevant API components may be missing
(4) it does not specify any order or compositional operators used to generate new pipelines from these components

Providing a weak specification allows a user to exert influence on the final pipeline produced, while at the same time not requiring deep API or machine learning expertise, as they do not have to manually detail the complete space. For example, a user can enforce a degree of interpretability on the optimized pipeline by writing a specification with a single linear model (e.g. logistic regression).

Definition 3.2. Strong Specification. Let h_c be a map from a subset of hyperparameters for component c to a collection of possible values. Let C be a map from component i to its respective h_i. Let P be a search procedure to generate candidate pipelines. A strong specification is a triple of the form $\langle C,(h_1,...,h_n),P\rangle$.

A strong specification, in effect, defines a search space for an AutoML tool. We propose that this space can be derived from the weak specification, which expresses (partial) user preferences.

In the following sections, we detail our approach to automatically strengthening weak specifications to influence the AutoML search process. But first, we introduce an illustrative scenario to demonstrate a use case for AMS.

4 ILLUSTRATIVE SCENARIO

We follow the journey of a forensic scientist who wants to classify glass fragments using a machine learning pipeline. In forensic science, glass fragments are used as an identifier when examining a suspect's clothing [9, 13]. The forensic scientist has a high level understanding of different learning and preprocessing algorithms. However, they are by no means an expert. They would not be aware of what kind of hyperparameters exist for different methods, nor what the impact of different parameter values could be on the pipeline's performance. They also are unaware if there may be other algorithms they should consider. The scientist has heard of AutoML and thinks this might be a suitable tool to explore pipelines. However, they have clear constraints: no tree-based ensemble models, as the pipelines need to be easily interpretable for downstream consumers such as detectives. Unfortunately, AutoML tools are known to often produce tree-based ensemble models [14, 20], which are challenging to interpret [21].

They spent some time on the internet and found a related paper that detailed a Scikit-Learn [38] pipeline that may work for their use case:

- `sklearn.preprocessing.PolynomialFeatures`
- `sklearn.preprocessing.MinMaxScaler`
- `sklearn.feature_selection.VarianceThreshold`
- `sklearn.linear_model.LogisticRegression`

The scientist will use this example pipeline (with no hyperparameters or values) as a weak specification for the kind of operations they would like to use. To evaluate their progress, they will use an existing classification dataset, "glass" [13], consisting of continuous measurements for 7 types of glass. The scientist performs a random 80/20 split for training/testing and evaluates pipelines using macro-averaged F1 score. The steps in this scenario and their resulting pipelines are summarized in Table 1.

The scientist starts by naively running the above mentioned specification directly as a pipeline with default hyperparameters, which results in an initial F1 score of *0.43*. Next the scientist uses the specification components, with default hyperparameters, as a configuration for the AutoML tool TPOT [36], which uses genetic programming to generate candidate pipelines. Applying TPOT to the weak specification (with no hyperparameters defined in the search space) results in a better score of *0.51*.

After consulting with a machine learning colleague, the scientist sets up a defined hyperparameter space (i.e. which hyperparameters to tune and set of possible values) for each component in the specification. The scientist then applies the same genetic programming search to the new configuration, resulting in pipeline number 2 in Table 1. Note that the shape of the optimized pipeline is the same as in the prior step, but now the regularization penalty and its weight varies. This step raised their score to 0.57.

Finally, the scientist recognizes that they may have missed additional components that could be helpful (their specification was based on a single paper, after all), and that the space of hyperparameters for their components should likely reflect common choices. They now use AMS, our approach, to automatically strengthen the initial weak specification rather than manually specifying the full space. AMS extends the specification using a code corpus and the API's documentation. Applying the same search procedure to AMS's specification now results in the highest score of *0.75*. The final pipeline retains polynomial features, but replaces the variance threshold selector with a selector based on a specified false positive rate. The pipeline then stacks a SGDClassifier (with hinge loss) and uses logistic regression with an L1 penalty (to produce sparse coefficients). This embodies the spirit of the initially given specification, but substantially outperforms the rest of the approaches.

5 AMS

We introduce AMS, a system that automatically strengthens weak pipeline specifications using an existing code corpus, an API's documentation, and an input search procedure. Figure 1 shows a diagram

#	Pipeline	Description	Score
1	PolyFeatures, MinMaxScaler, VarianceThreshold, LogisticRegression	Initial (naive) weak specification as a pipeline with default hyperparameters.	0.43
2	StackingEstimator(LogisticRegression), LogisticRegression	Applying AutoML tool TPOT (Genetic Programming) to the original specification without defining any hyperparameters.	0.51
3	StackEstimator(LogisticRegression ([Penalty: L1, Cost: 10]), LogisticRegression	Same as #2, but with expert-defined hyperparameter space for regularization (cost) and penalty.	0.57
4	PolyFeatures, SelectFPR, StackingEstimator(SGDClassifier [Loss: Hinge]), LogisticRegression [Penalty: L1, Cost: 100]	Applying genetic programming to the strong specification generated by our approach (AMS) given the weak specification.	0.75

Table 1: Summary of scenario iterations based on the "glass" dataset showing the progression of score improvements. The first pipeline runs the (naive) weak specification directly. The second and third pipelines are produced by applying a genetic programming search to the original specification and a variant with an expert-defined hyperparameter space, respectively. The fourth (and highest scoring) pipeline is produced by transforming the weak specification to a strong specification using our approach, AMS, and applying the same genetic programming search procedure.

of the system. AMS takes the user's weak specification as input. The system first extends the set of API components considered in the specification. To perform this extension, AMS relies on a code corpus, which exercises the target API, and on the API's natural language documentation. After the specification has been extended, AMS uses the code corpus to identify key hyperparameters for the API components in the specification and include sets of possible values they can take on. AMS then pairs this set of component configurations with a search procedure to produce a strong specification. The search procedure can then be used to iteratively sample and evaluate candidate pipelines, resulting in a final optimized pipeline.

We now present details on each step in the AMS system.

5.1 Discovering Unspecified but Useful API Components

AMS first extends the initial specification with additional components, which the user may not have included. Given a specification S and a new component c, c may be added to S if it satisfies one of the following two conditions:

- c is commonly used with a component already in S.
- c could replace a component already in S.

The goal of the first condition is to identify *complementary components*. For example, if a classifier is often used with a particular preprocessing step, we say these components are complementary. The goal of the second condition is to identify *functionally related* components, which are alternatives to each other. For example, two different linear classifiers would be considered functionally related alternatives to each other.

AMS relies on two different sources of information to identify components that satisfy each of these conditions. We first address complementary components.

5.1.1 Complementary Components. To identify complementary components, AMS exploits information from a crowd-sourced corpus of scripts, which exercise the target API. Each script in the corpus was written to target a single dataset, therefore two components used in the same script may be complementary. By using a code corpus to identify such components, AMS can automatically produce and update its inventory of complementary components to reflect current ML practices.

From the code corpus, the system extracts all scripts that contain a call to our target API library and records the set of API components used in each script. The intuition is that these sets can be used to measure the likelihood of components co-occurring, and that complementary components must (by definition) co-occur more frequently.

Formally, we compute the normalized pointwise mutual information (NPMI) [5] over the collection of all (unordered) pairs of co-occurring API calls in our code corpus to identify complementary components. Let X and Y be two random variables, defined over the the domain of our target API library, NPMI for two components x and y is defined as

$$\text{NPMI}(x,y) = \frac{\log_2\left(\frac{p(x,y)}{p(x)p(y)}\right)}{-\log_2(p(x,y))} \tag{1}$$

where $p(x)$ is the fraction of pairs where either element is x divided by the number of all pairs, similarly for $p(y)$, and $p(x,y)$ is the fraction of pairs (x,y) or (y,x) divided by the number of all pairs.

NPMI ranges between -1 and 1, where -1 means the components never co-occur, 1 means the components always co-occur, and 0 means the components are independent. We compute the NPMI over the set of all pairs of co-occurring components (i.e. API components called in the same script). Eliminating pairs with an NPMI less than or equal to zero yields pairs of varying degree of complementarity.

When given a weak specification, we can identify all NPMI-positive pairs that share a component with the specification. For each such pair, the new potential component corresponds to the element in the pair that is not in the original specification. If more than one component in the original specification support (i.e. co-occur with) a new component, we compute an average NPMI. For each possible new component, we compute a weighted sum of the average NPMI and the fraction of original specification components that support it. The weighted sum balances average NPMI and support fraction based on a user-defined weight $\alpha \in [0,1]$. We then take the top K_{comp} new components and add them as complementary components to the original specification. Algorithm 1 describes this procedure.

5.1.2 Functionally Related Components. The goal of identifying functionally related components is to include algorithm alternatives in the specification. For example, the user's weak specification may indicate that they are interested in using linear models, but they may have not exhaustively listed all linear model alternatives. This task raises the challenge of reasoning about the semantics of API components. Rather than reason about component semantics, we rely on a simpler notion of similarity.

Algorithm 1 Extracting Complementary Components

INPUT: A collection P of unordered pairs of co-occurring API components extracted from a code corpus; a function NPMI that computes the normalized pointwise mutual information of two API components; a specification $S = \{c_1, \ldots, c_n\}$; a weight $\alpha \in (0, 1)$ to combine NPMI and support fraction; and an integer K_{comp} for the maximum number of complementary components to take.

OUTPUT: A new specification S' extended with at most K_{comp} new components.

procedure ComplementaryComponents
- ▷ *Map from co-occurring pair to accumulator list of NPMI scores*
- npmis ← {}
- **for** $c \in S, (p_1, p_2) \in P$ **do**
  - **if** $(c \in (p_1, p_2)) \wedge (p_1 \notin S \vee p_2 \notin S)$ **then**
    - new ← p_2 if $c_1 = p_1$ else p_2
    - ▷ *Accumulate the npmi score*
    - npmis[new] ← npmis[new] :: NPMI(p_1, p_2)
- ▷ *Compute average npmi and support fraction*
- ▷ *Combine using α to create score*
- scores ← {}
- n ← LEN(S)
- **for** comp ∈ npmis **do**
  - vals ← npmis[comp]
  - scores[comp] ← AVG(vals) $* \alpha +$ $\left(\frac{\text{LEN(vals)}}{n}\right) * (1-\alpha)$
- S' ← $S \cup$ GETTOPK(scores, K_{comp})

We would like to define a function SIM(c_1,c_2) that computes a score for two API components, c_1 and c_2, such that a higher score corresponds to higher degree of semantic similarity. Given a component c_i, we can then sort all possible components in our target API in descending order based on their similarity score with respect to c_i.

AMS exploits the fact that the target library has natural language documentation for each component (as part of its developer documentation), which we assume details key aspects about their functional behavior. By mining the API's documentation, AMS can be used to automatically identify functionally related components in new target libraries or new versions of previously used libraries without the need for extensive expert annotation.

We define SIM(c_1,c_2) to compute over the documentation[2] for c_1 and c_2 and we instantiate SIM to use a classical relevance/similarity scoring technique: BM25 [41]. BM25, detailed below, produces a score for a document, given a query and a corpus of documents. A higher score indicates a higher degree of lexical correlation between the document and the query.

$$\text{BM25}(D,Q) = \sum_{i}^{n} \text{IDF}(C,q_i) \frac{f(q_i,D) * (k_1+1)}{f(q_i,D) + k_1 * \left(1 - b + b * \frac{\text{LEN}(D)}{\text{AVGLEN}(C)}\right)} \tag{2}$$

where D is a document, $Q = (q_1,\ldots,q_n)$ is a query comprised of q_i terms, C is a corpus of documents, and k_1 and b are score hyperparameters[3].

[2]We perform standard preprocessing of the documentation strings such as tokenization, stemming, and extension with the path of the given component in the library's module structure.

[3]We use the gensim [40] BM25 implementation, where $k_1 = 1.5$ and $b = 0.75$ are implementation-defined constants.

In our setting, the documentation for an existing component in the weak specification corresponds to the query, a particular API component's documentation corresponds to the document, and the entirety of the API's documentation corresponds to the document corpus.

AMS uses SIM to retrieve, and append, the top K_{rel} new components for each component in the original weak specification (i.e., we do not consider any complementary components added for purposes of this procedure). Algorithm 2 describes this procedure.

Algorithm 2 Extracting Functionally Related Components

INPUT: A collection C of API components; a map M from API component to documentation; a function SIM that computes the BM25 score between a query string and a document; a specification $S = \{c_1, \ldots, c_n\}$; and an integer K_{rel} for the maximum number of complementary components to take per component in S.

OUTPUT: A new specification S' extended with at most K_{rel} per component in the original specification.

procedure FunctionallyRelatedComponents
- ▷ *Set of empty API components*
- extension ← $\emptyset$
- **for** $c \in S$ **do**
  - scored ← $\{(c', \text{SIM}(M[c], M[c'])) \text{ for } c' \in C \text{ if } c' \notin S\}$
  - c_K ← GETTOPK(scored, K_{rel})
  - extension ← extension $\cup c_k$
- S' ← $S \cup$ extension

5.2 Identifying Hyperparameters and Values

Machine learning practitioners often spend a significant amount of time not just choosing pipeline components, but also tuning the hyperparameters associated with each component. Performance can significantly increase by identifying the appropriate hyperparameter values for a given dataset and pipeline [39].

AMS relies on the corpus of scripts that make calls to the target API to identify the set of relevant hyperparameters and possible values. This design choice hypothesizes that an AutoML system should focus on tuning the set of hyperparameters and hyperparameter values that human developers focus on tuning.

For each script in our code corpus that imports the target API, we parse the source code and identify calls to API class constructors. We extract the set of optional arguments in each constructor call and record each (argument name, argument value) as a hyperparameter setting. The value recorded corresponds to a constant in the call, or points to an unknown placeholder.

When given a specification, AMS takes each API component and identifies the set of top K_{params} hyperparameter names observed in the mined code for that component, along with the top K_{vals} values observed for each of the names. AMS adds the default value for each hyperparameter to the set of possible values (obtained by introspecting the class definition), and then emits this as the corresponding hyperparameter search space. Algorithm 3 describes this procedure.

Figure 2 shows a specification extended with a complementary component (Algorithm 1), a functionally related component (Algorithm 2), and hyperparameters and values (Algorithm 3).

Algorithm 3 Adding API Component Hyperparameters and Values

INPUT: A map P from API components to hyperparameter names and frequencies observed in calls; a map V from hyperparameters to values and their frequencies observed in calls; a specification $S = \{c_1, \ldots, c_n\}$; an integer K_{params} for the maximum number of hyperparameters to consider per component; and an integer K_{vals} for the maximum number of values per hyperparameter to consider.

OUTPUT: A new specification S' with at most K_{params} hyperparameters per component and at most $K_{\text{vals}}+1$ (including default value) per hyperparameter.

```
procedure HyperParamsAndValues
    ▷ Empty map from component to hyperparameter space
    S' ← {}
    for c ∈ S do
        params ← GetTopK(P[c], K_params)
        ▷ Empty configuration for component c
        c_config ← {}
        for p ∈ params do
            values ← GetTopK(V[p], K_vals)
            ▷ Append default value, if not included
            values ← values :: GetDefaultValue(p)
            c_config[p] ← values
        S'[c] ← c_config
```

```
{ # original weak spec -- just component
'sklearn.linear_model.LogisticRegression': {
  'C': [100000.0, 7, 1.0],
  'penalty': ['l1', 'l2']
},
# complementary component
# (only called with defaults in our corpus)
'sklearn.feature_extraction.text.TfidfTransformer': {},
# functionally related component
'sklearn.linear_model.SGDClassifier': {
  'loss': ['log', 'hinge'],
  'penalty': ['l2', 'elasticnet']
} }
```

Figure 2: A weak specification extended with one complementary component, one functionally related components, and two hyperparameters/values per component (plus a potential default value, if different).

5.3 Search Procedure

To fully satisfy the definition of a strong specification, AMS must add in a specific search procedure to the extended specification. AMS allows the use of different search procedures, which can be plugged into the system. In particular, the current implementation of AMS presents a plug-in genetic programming search procedure, implemented in an external tool, and a conceptually simple random search procedure implemented as part of AMS's codebase.

5.3.1 Genetic Programming. We use TPOT [36], a genetic programming based AutoML tool, as a search procedure. When using TPOT, we use the search space defined by AMS as the configuration available to the optimization process.

5.3.2 Random Search. AMS's implementation includes a hierarchical random search procedure to generate sequential (i.e. API components are chained in sequence) pipelines. Random search is known to perform better for algorithm configuration than equally simple alternatives such as grid search [4] and has also been successfully applied to related software engineering areas such as product line configuration [34]. To generate a pipeline, the search module samples a depth (up to a bound), then for each step in the pipeline it samples an API component from the configuration specified. For each hyperparameter in the chosen component's configuration, the search samples a value and sets it in that component's constructor. The search distinguishes between preprocessing and classifier components to generate valid candidate pipelines (i.e. the last step must always be a classifier). Candidate pipelines are cached to avoid re-training/evaluating pipelines, however, there is no effort to exhaustively search the space and if a pipeline is re-sampled a given number of times (100 in our implementation), the search procedure terminates.

6 EVALUATION

We now present our experimental results, which evaluate individual parts of our system (RQ1-RQ3) and the overall performance of AMS (RQ4). First, we characterize the complementary API components extracted from our code corpus (RQ1). We evaluate AMS' ability to retrieve functionally related API components (RQ2). We then characterize the use of hyperparameters and their values in our code corpus, and evaluate the possibilities for improving classifier performance based on this information (RQ3). Finally, we evaluate AMS's ability to produce specifications that result in higher performance (RQ4).

For our evaluation, we implemented AMS and its evaluation in approximately 4500 lines of Python. We use Scikit-Learn [38], a popular Python machine learning library, as the target API for pipelines. To mine complementary components and identify hyperparameters/values, we use the meta-Kaggle [27] dataset as our code corpus. The meta-Kaggle dataset contains over 3300 Python scripts.

6.1 RQ1: Complementary API Components

AMS mined 285 normalized PMI (NPMI) positive association pairs from our code corpus. These associations cover 69 different components (39.2% of all components in Scikit-Learn).

Table 2 details the distribution of associations based on the algorithmic role of each of the components, along with their mean and standard deviation NPMI.

To evaluate the effectiveness of these NPMI-based component extensions, we conduct the following experiment. We take each script in our code corpus, and extract the set of Scikit-Learn components used. Using 10-fold cross validation (CV), we split this collection of components into a training fold and test fold. We use each training fold to compute NPMI, and we use the corresponding test fold to evaluate. For each set (ground truth) in the test fold, we take each component individually and use it as a query term to retrieve the top $K_{\text{comp}} \in [1,5]$ complementary components based on our approach (Algorithm 1, with $\alpha = 0.5$). We then compute precision as the fraction of retrieved components that are present in the full ground truth component set. Note that recall is not an appropriate measure of performance for evaluating complementary components, as recall implies our extensions need to be complete, but by definition we will only be able to cover components with strong co-occurrence patterns. Given this, we focus on precision.

Rule Type	# Rules	Mean Norm. PMI	SD Norm. PMI
classifier	78	0.18	0.11
(classifier, cluster)	1	0.37	-
(classifier, decomposition)	3	0.16	0.13
(classifier, feature extraction/selection)	29	0.19	0.15
(classifier, preprocessor)	31	0.20	0.13
(cluster, decomposition)	2	0.45	0.26
(cluster, preprocessor)	1	0.27	-
(cluster, regressor)	3	0.10	0.05
(decomposition, feature extraction/selection)	7	0.17	0.19
(decomposition, preprocessor)	4	0.24	0.26
(decomposition, regressor)	3	0.20	0.25
feature extraction/selection	3	0.35	0.25
(feature extraction/selection, preprocessor)	10	0.25	0.20
(feature extraction/selection, regressor)	4	0.17	0.12
preprocessor	3	0.32	0.26
(preprocessor, regressor)	6	0.20	0.21
regressor	97	0.19	0.07

Table 2: NPMI-based association rules mined from our code corpus to identify complementary API components categorized by algorithmic role. When both components in the association have the same role, we elide one for brevity.

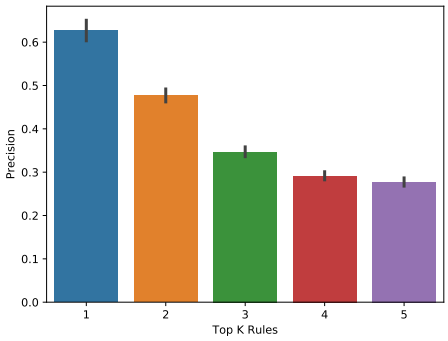


Figure 3: Precision of NPMI-based component extension on our code corpus. Using 10-fold CV, we sample a component from a set, use this as a query term, and evaluate the precision of the returned extensions (for varying K_{comp}) by comparing to the original complete set. Our NPMI-based approach can produce at least one complementary component for 82.68% of our test observations, with precision of approximately 60% when $K_{\text{comp}} = 1$.

We found that 82.68% of the sets in the test folds were covered (i.e. we were able to identify at least one complementary component). For $K_{\text{comp}} = 1$, we found that our NPMI-based approach yields a precision of 60%. This precision declines, as expected, when we increase K_{comp}, with a precision of approximately 28% when $K_{\text{comp}} = 5$. Based on these results, we configured AMS to use $K_{\text{comp}} \leq 3$. Figure 3 summarizes these results.

6.2 RQ2: Functionally Related API Components

To evaluate AMS's retrieval of functionally related components, we manually annotated our BM25-based ranking of API components for a given query component. To determine if two components were functionally related, we outlined a set of conditions that they should satisfy. Given a specification component Q (for query) and a possible extension component R (for related), we say they are functionally related if they satisfy the following:

- R could replace Q in a pipeline without raising an exception for the same dataset.
- Q and R belong to the same class of operators (e.g. classifier, regressor, value normalizer, decomposition algorithm, loss function).
- If Q/R are classifiers/regressors, they must respect output shape constraints: a multi-task model can replace a single task model, but not vice-versa.
- If Q is (non-)linear, R must be always (non-)linear or must be (non-)linear based on a hyperparameter (e.g. SVM with a linear kernel)
- If Q is ensemble-based, R must be ensemble-based with one exception: R can be non-ensemble based if it is related (based on these rules) to the weak model class ensembled in Q.
- If Q is not ensemble-based, R may be ensemble-based if it uses a weak model class related to Q to create its ensemble.

To carry out our experiment, we randomly sampled 50 classes from Scikit-Learn and used these as queries. We chose to sample 50 classes as this covers approximately 28% of the components available in Scikit-Learn and balanced the need for detailed manual annotation. For each query, we retrieved the top 10 API components based on: 1) our BM25 metric, 2) cosine similarity using averaged pre-trained neural embeddings (which have been shown to be effective for the related task of code search [6]), and 3) a uniform random metric. We used (2) to compare the use of BM25 with another unsupervised approach to semantic similarity. We used BERT embeddings derived from a scientific text corpus [3]. We used (3) as a baseline to control for the extent to which our target API (Scikit-Learn) may have redundant components resulting in functionally related results through chance.

Figure 4 presents our results. The BM25-based ranking performed comparably (with no statistically significant difference) to the embeddings based approach. A random ranking results in approximately 10% functionally related results, across the top 1, 5, and 10 query results. In contrast, BM25 results in close to 72%, 55%, and 44% functionally related results across the same cutoffs, respectively. We opted to use BM25 in AMS, in contrast to the neural embeddings approach, given their comparable performance and the added advantage of avoiding the additional storage requirements imposed by per-token embeddings.

Note that while for purposes of this experiment, we allow functionally related components to include ensembled-variants of non-ensemble models, in our tool implementation users can exclude ensembles through a simple command line flag.

6.3 RQ3: Hyperparameters and Values

Figure 5 characterizes the hyperparameter tuning observed in our code corpus. In particular, we found that over 50% of the calls tune (i.e. explicitly set a value in the call) for under 20% of the hyperparameters available (5a); for about a third of API components the set of hyperparameters tuned is similar across calls (5b); and for over 70% of the hyperparameters observed, user calls choose few values (under 10 distinct values) (5c). This aligns with our intuition that human developers tend to tune a small set of hyperparameters, these

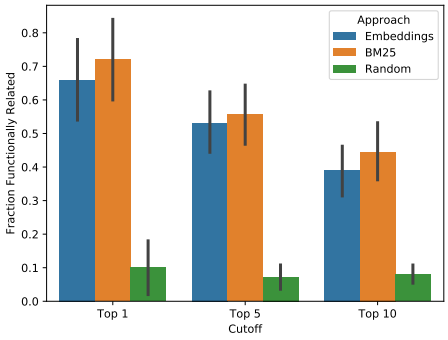


Figure 4: For 50 randomly sampled query API components, BM25 can retrieve close to 72%, 55%, and 44% functionally related components based on top 1, 5, and 10 cutoffs, respectively. Based on our criteria, BM25 performs slightly better (on average) than another unsupervised approach using averaged BERT embeddings.

are consistent across datasets/pipelines, and there are popular values that developers choose for each.

To demonstrate the possible impact of hyperparameter tuning, we performed the following experiment. We collected five datasets from the Penn Machine Learning Benchmarks (PMLB) [37]. The five datasets are healthcare-related classification tasks. We collected these 5 dataset to be independent from those used in RQ4. We then identified the top 5 most common classifiers[4] from our code corpus. For each classifier, we extracted the top 3 hyperparameters and top 3 values for each hyperparameter, along with the default values. We performed grid search over these values to evaluate all possible configurations. We then compared the best macro-averaged F1 score [16] from the grid search with the score obtained under the default configuration.

Figure 6 shows our results. In almost all cases, the hyperparameter space defined by the code examples in our corpus contained a setting which would have improved performance with respect to the default configuration. For the ensemble-based classifiers, ExtraTreesClassifier and RandomForestClassifier, this improvement could have been up to 10% on two of the datasets.

6.4 RQ4: Performance of Strong Specifications

We now describe the experimental setup used to evaluate the overall performance of AMS.

Our experiments compare the following approaches:

- Weak Spec.: runs an ordered version of the original weak specification as a pipeline directly.
- Weak Spec. + Search: carries out a specified search procedure over the components defined in the weak specification (with default hyperparameters).
- Expert + Search: uses the set of hyperparameters and possible values defined in TPOT's default classifier configuration [2] for each component in the specification. We apply the specified search procedure over this space of components and hyperparameters. This choice of hyperparameter space corresponds to an expert AutoML developer identifying key hyperparameters and values. We also evaluated writing our own hyperparameter space and found that it performed comparably or worse, so we elide for brevity.
- AMS + Search: applies AMS to the weak specification to produce a full search space and then applies the specified search procedure.

[4] excluding SVM, which did not terminate within a reasonable computing budget without additional data pre-processing for these datasets

Short name	Component
lr	Logistic Regression
rf	Random Forest
dt	Decision Tree
scale	Min-max value scaling
poly	Extract polynomial features
var	Variance-based feature selection
pca	PCA decomposition

Table 3: Components used to produce weak specifications for evaluation. When evaluating the *Expert + Search* approach, we take the hyperparameter search space defined in TPOT's default classifier configuration for the corresponding component. This choice of hyperparameter space reflect those of an expert AutoML developer.

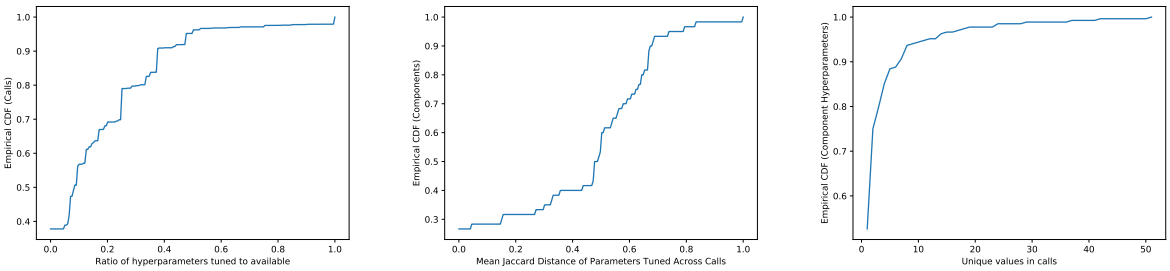
For these experiments, we consider both search procedures available in AMS: genetic programming and random search.

Table 3 presents the individual components used to create the weak specifications for our experiments. We chose components that covered common machine learning operations: value scaling, feature derivation, feature selection, dataset decomposition, and varied forms of classification. For each such component, we also outline a subset of hyperparameters identified for tuning and their possible values, which are used in the *Expert + Search* approach.

We produced 15 weak specifications by combining the following 5 pre-processing weak specifications with each of the three classifiers (lr, rf, dt) - as outlined in Table 3: {} (no-preprocessing), {scale}, {poly, scale}, {poly, scale, var}, and {poly, scale, pca, var}.

For our experiments we used all classification datasets from the original TPOT paper [36]; 9 in total. These datasets are: Hill-Valley-with-Noise, Hill-Valley-Without-Noise, breast-cancer-wisconsin, car-evaluation, glass, ionosphere, spambase, wine-quality-red, and wine-quality-white. All datasets are available through PMLB [37]. We refer the interested reader to the TPOT paper for more details on each dataset.

Our experiments used macro-averaged F1 score as a performance metric, where a higher score corresponds to better performance. Each search procedure uses this same score metric in their internal search loop. For each benchmark, dataset, and search procedure combination, we carried out 5-fold CV with each of the approaches outlined previously. In each cross-validation iteration, the training fold is used to find an optimized pipeline, and the test fold is used for evaluation. All approaches were provided a budget of 5 minutes per CV iteration (i.e. 25 minutes per dataset, for each specification and approach combination).



(a) Fraction of hyperparameters tuned **(b) Distance between sets of hyperparameters tuned** **(c) Unique values used for a hyperparameter**

Figure 5: Characterizing hyperparameter tuning in our code corpus.

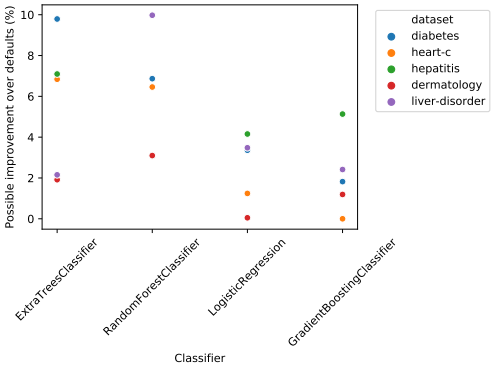


Figure 6: Possible improvements in performance (macro-averaged F1 score) by using hyperparameter settings identified in our code corpus, compared to the performance using default hyperparameter values.

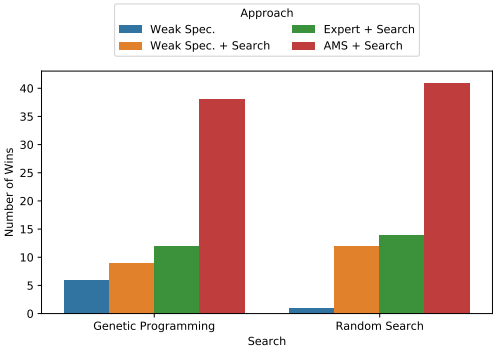


Figure 7: Wins for each approach across all 15 weak specifications, 9 datasets, and 2 search procedures, totaling 270 experiments. Within a given search procedure, a approach *wins* when it obtains the highest average 5-fold CV test-fold performance for a dataset and weak specification combination, *and* this score is at least 1% higher (in absolute terms) than the next best score.

We evaluate AMS with the following configuration: a weak specification can be extended with at most 3 complementary components ($K_{\text{comp}} = 3$), where the npmi/support fraction weighing parameter is set to 0.5 ($\alpha = 0.5$), for each specification component we include up to 4 functionally related components ($K_{\text{rel}} = 4$), and we tune the top 3 hyperparameters per component ($K_{\text{params}} = 3$) by choosing from the 3 most common values per hyperparameter ($K_{\text{vals}} = 3$). We set the depth bound for the random search procedure to 4.

Figure 7 presents a count of the wins for each approach across both search procedures [8]. An approach *wins* when the average of the 5-fold CV test-fold performance metric is the highest across approaches for a given dataset and weak specification combination, *and* the score is at least 1% (in absolute terms) higher than the next best score. We introduced a minimum performance difference threshold to eliminate cases where multiple approaches perform roughly equally on a specification/dataset combination. We varied the minimum difference threshold from 1% to 5% (absolute) and found that AMS obtained more wins than other approaches in all cases.

When using genetic programming as a search procedure, we see that *Weak Spec.* obtained 6 wins compared to 9 wins for *Weak Spec. + Search*. Under random search, *Weak Spec.* obtained 1 win and *Weak Spec. + Search* obtained 12 wins. *Expert + Search* obtained 12 wins when using genetic programming, and 14 wins when using random search. Under both search procedures, using AMS produced the majority of wins: 38 in the genetic programming experiments and 41 in the random search experiments.

Figure 8 presents the distribution of the top-10 Scikit-Learn operators as a fraction of the total count of operators in pipelines produced by genetic programming using AMS's strengthened specification for two different weak specifications. For comparison, running genetic programming over the full search space (as defined in TPOT's default classification configuration) produces pipelines where 60% of them have an ensemble-based model (one of GradientBoosting, ExtraTrees, XGBoost, or RandomForest), and at least one pipeline produced in 8 of the 9 datasets includes such a component. The skew towards ensemble-based models has been observed in other AutoML tools as well [14]. By using AMS a user can restrict the use of ensemble-based models, for example, if desired.

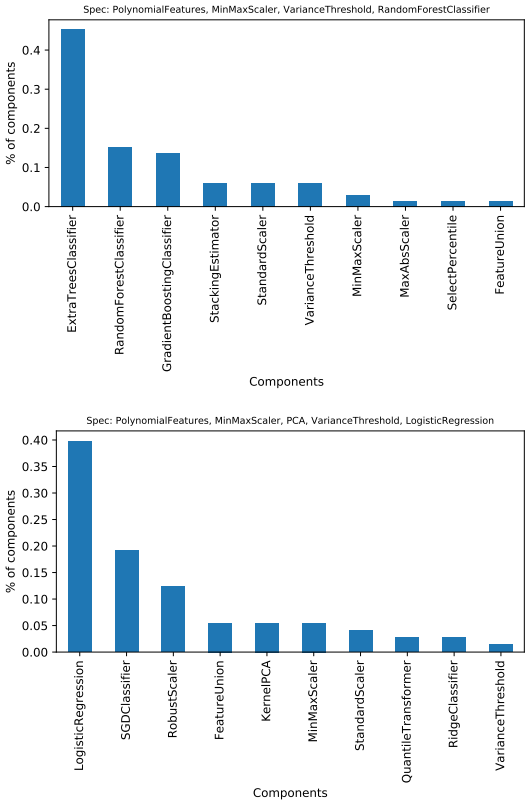


Figure 8: Example distributions of Scikit-Learn components in pipelines produced by genetic programming, based on AMS strengthening of the initial weak specification.

7 RELATED WORK

We address prior research related to AMS in three main areas: automated machine learning, search-based software engineering, and code mining.

Automated machine learning (AutoML) has received increased attention in the recent past. TPOT [36] uses genetic programming to automatically produce tree-structured classification and regression pipelines composed of Scikit-Learn [38] operators. Autosklearn [15] uses sequential model-based algorithm configuration (SMAC) [25] to generate Scikit-Learn pipelines and their hyperparameter settings. ReinBo [43] uses reinforcement learning to generate pipeline candidates and Bayesian optimization to tune their parameters. AL [7] learns a pipeline likelihood model from dynamic program traces and uses this to generate sequential Scikit-Learn pipelines, with default hyperparameter values. In contrast to these systems, AMS focuses on providing AutoML users with a simple way of influencing the pipeline generation process: writing a weak specification, which can be automatically strengthened. This usage model empowers users to influence pipeline generation on a per-specification basis, rather than relying on distributional characteristics of a pipeline corpus (as in AL), on the developer pre-defined search spaces in the original AutoML tool (as in TPOT, ReinBo and Autosklearn), or manually specifying a new complete search space that reflects their preferences (as in TPOT's optional configurations).

TPOT can take in a configuration that indicates the set of API components and possible hyperparameters/values for use during search. The TPOT developers provided three pre-defined configurations: "TPOT light" for fast operators that can scale to larger datasets, "TPOT MDR" for genomic studies [29], "TPOT sparse" for sparse datatypes, and "default" [1]. The variety of different configurations highlights the need for expressing pipeline preferences. AMS can be used to produce such configurations automatically, on an ad-hoc basis (without expert developers' involvement), for varied user needs. For example, a user can bias the output pipeline away from tree-based ensemble models, which are known to have high predictive accuracy but complicate interpretability [21].

Search-based Software Engineering (SBSE) [22] provides a general framework through which to design and analyze AutoML systems, with the latter effectively being a instance of the former. SBSE has been successfully applied to problems such as automated testing of software with large test suites [31], synthesizing equivalent method call sequences [19], and optimizing product line configurations [34], among others. AMS allows users to approach AutoML in a grey-box setting, where their weak specification can influence the search process. Feedback of this form can enable an *"iterative process of refinement"* [22] to obtain solutions that satisfy user preferences.

Code corpora have enabled advances in various areas of software engineering. Large-scale corpora that exercise particular APIs can be used to mine preconditions for method calls [32]. Code idioms mined from a corpus can be used to improve program synthesis and semantic parsing [42]. Semantic code search [6, 24] leverages a large-scale code corpus to answer developer queries. Particularly relevant for our system, query extension has been shown to improve search results when queries are underspecified [30]. AMS mines a code corpus to obtain complementary and functionally related API components, which can extend (and thus strengthen) the initial specification. AMS also relies on the code corpus to identify common hyperparameters and their values, used to refine the pipeline search space.

8 THREATS TO VALIDITY

We discuss potential limitations of this research based on design choices. In particular, we focus on threats to generalizability. First, our evaluation uses a particular ML framework (Scikit-Learn) and core corpus (meta-Kaggle). We believe this threat is mitigated by the fact that Scikit-Learn is a widely-adopted ML library, used by over 92,000 GitHub repositories as of March 2020. Similarly, code in the meta-Kaggle corpus represents a wide range of scripts written by different users targeting different datasets. Our evaluation only considered two search procedures: genetic programming and random search. Other search procedures may potentially find pipelines with different characteristics and performance. However, both random and genetic search are commonly used methods in search-based software engineering and have shown good performance over a wide range of AutoML problems. The choice of evaluation datasets could also influence our results. We used the classification datasets from the original TPOT paper, which have also been used in the evaluation of existing AutoML research [8, 10]. Finally, the weak specifications in our evaluation are naturally a sample of possible specifications. However, we aimed to incorporate common operations and components in these specifications to reflect standard usage.

9 CONCLUSION

We introduced a new usage model for AutoML systems, where a user provides a set of API components as a weak specification for a pipeline and this specification can be automatically strengthened. Introducing the notion of specifications enables users to exert control and express preferences over the resulting pipeline. It allows them to enforce the presence of certain properties, such as a degree of interpretability on the optimized pipeline by writing a specification with a single linear model (e.g. logistic regression). We implement our strengthening approach – extending the specification with complementary components using normalized pointwise mutual information on an existing code corpus, functionally related components using a lexical similarity score over the target API's documentation, frequency distributions on constructor calls in the code corpus to extract key hyperparameters and values, and a search procedure – in the AMS system. We evaluated AMS on a collection of 9 datasets and 15 weak specifications using two different search procedures. We show that the pipelines produced using AMS's strengthened specifications can outperform pipelines produced using the initial weak specifications and variants of the initial specifications annotated with expert-defined hyperparameter spaces.

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