{AMS}: Generating AutoML search spaces from weak specifications

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Team

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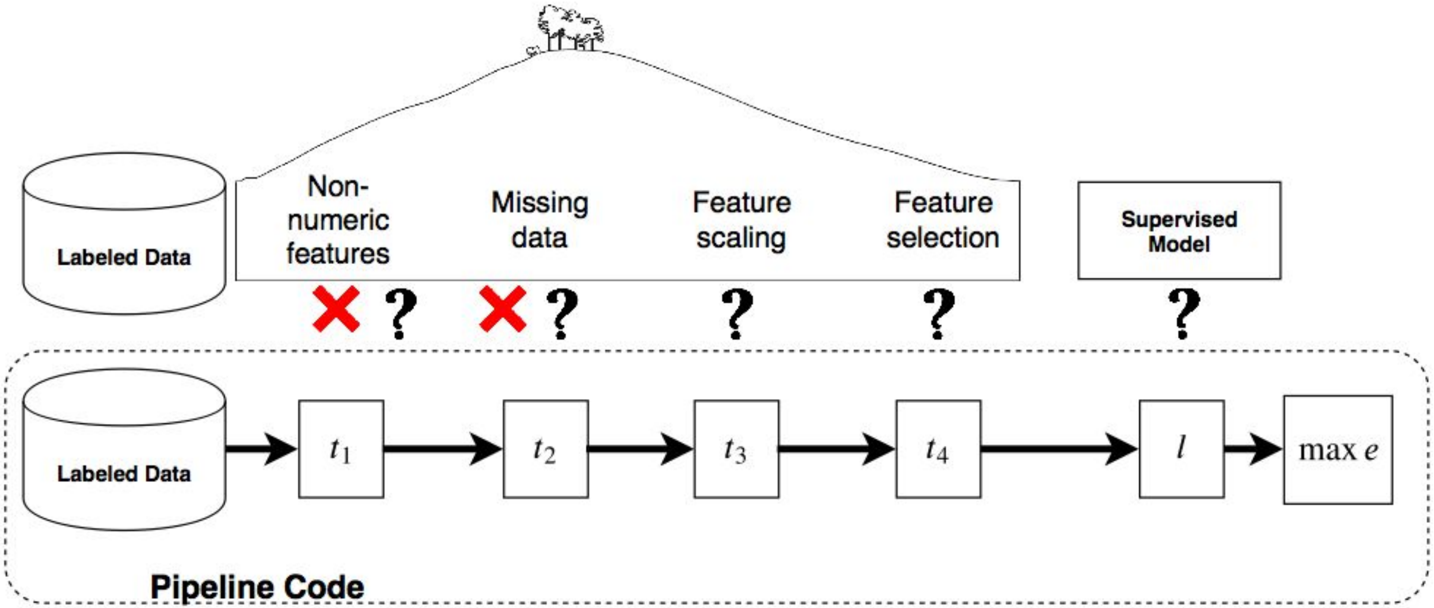
Machine Learning Pipelines



How can developers write ML pipelines?

Expert knowledge

Non-ML expert

ML Expertise Spectrum

How can developers write ML pipelines?

Manually implement and validate your own pipelines

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How can developers write ML pipelines?

Manually implement and validate your own pipelines

Use AutoML

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Pros/Cons of Manual/AutoML

- Manual
    - ✅ High degree of control
    - ❌ Requires expert knowledge
    - ❌ Developer-time consuming

Pros/Cons of Manual/AutoML

- Manual
  - ✅ High degree of control
  - ❌ Requires expert knowledge
  - ❌ Developer-time consuming
- AutoML
  - ❌ Low degree of control
  - ✅ Does not require expert knowledge
  - ✅ Reduces developer-time

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{AMS}

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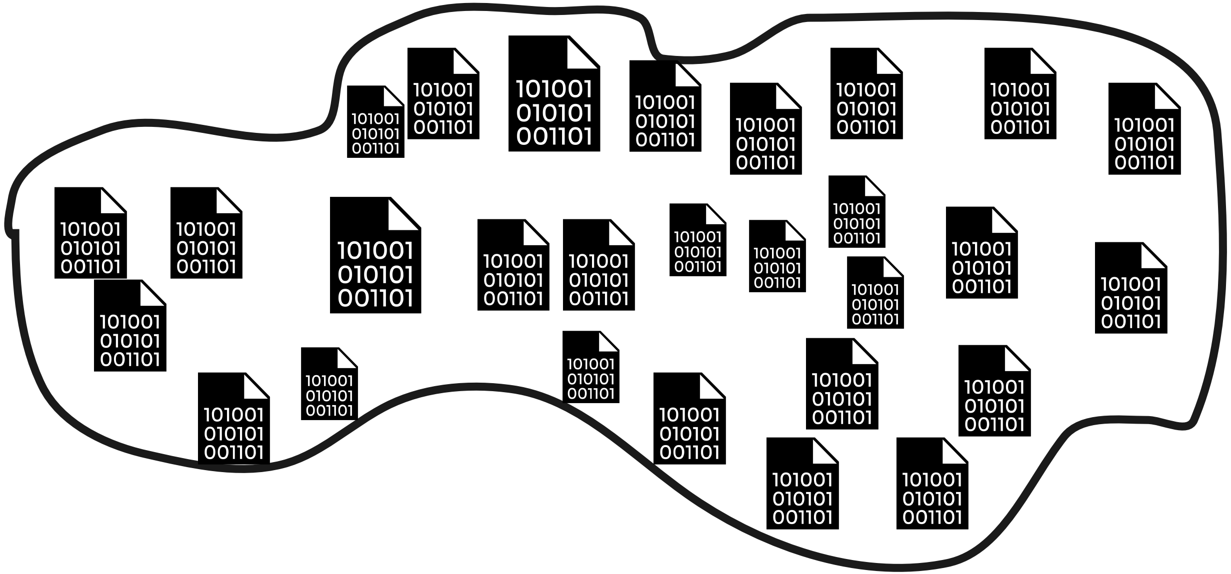
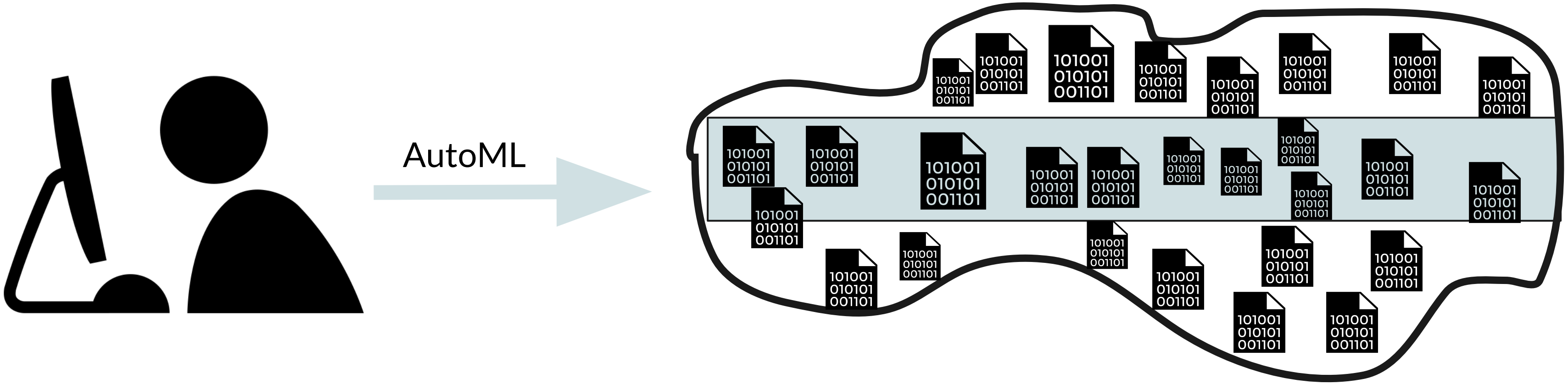
ML Pipeline Search Space



ML Pipeline Search Space



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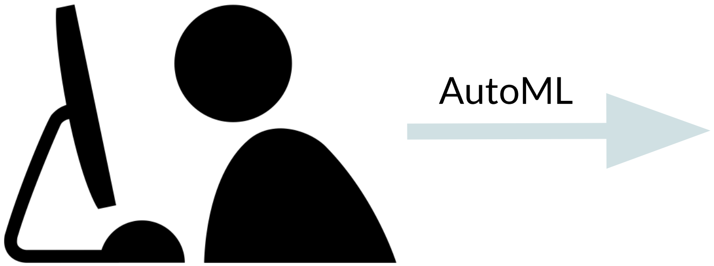

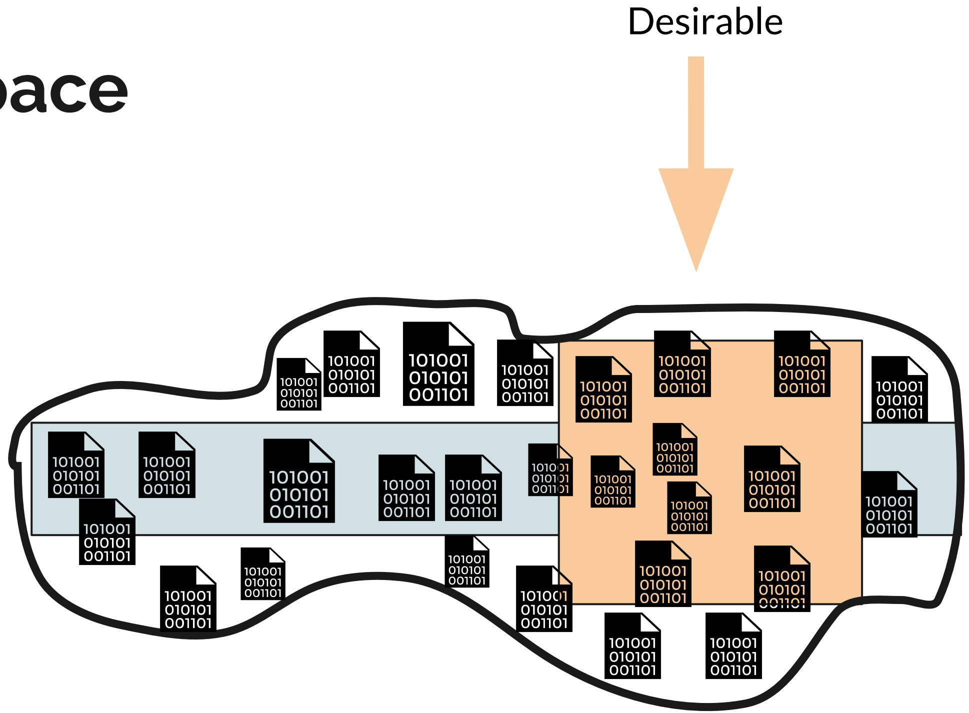

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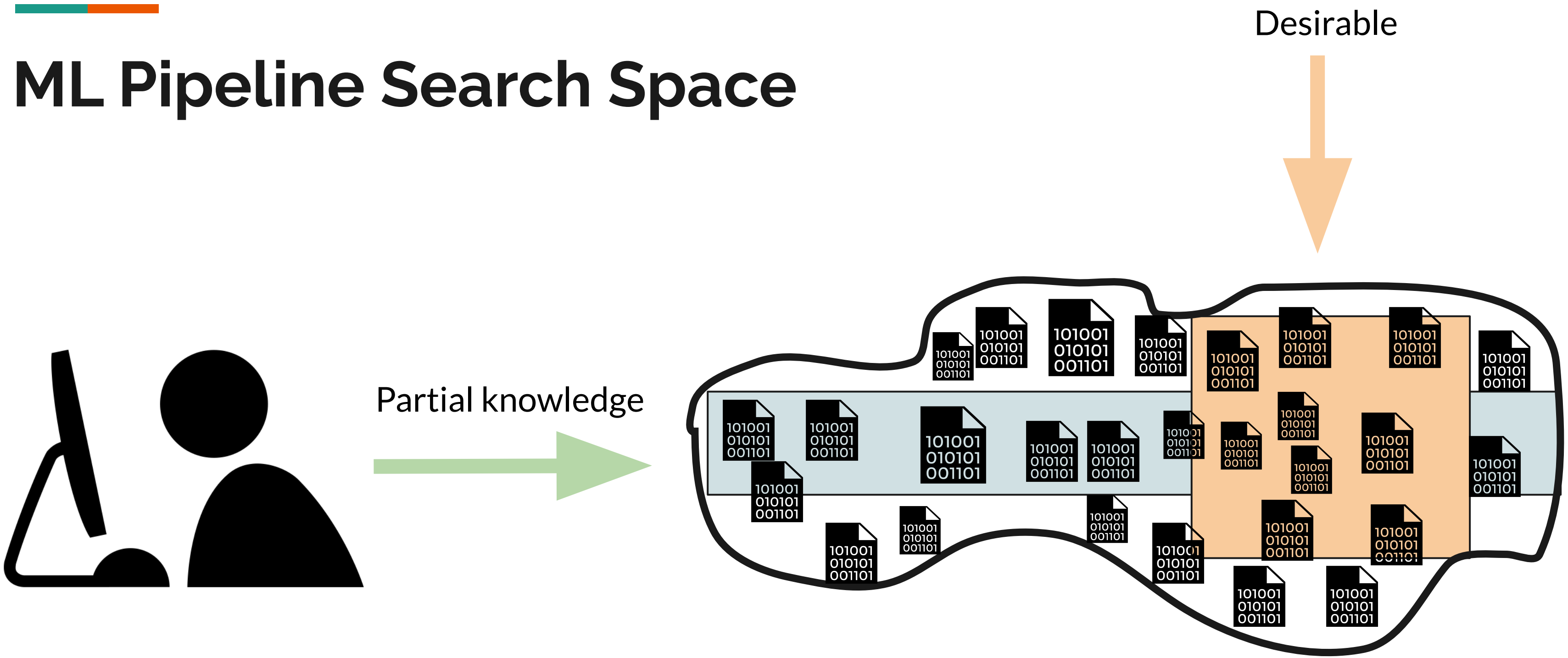

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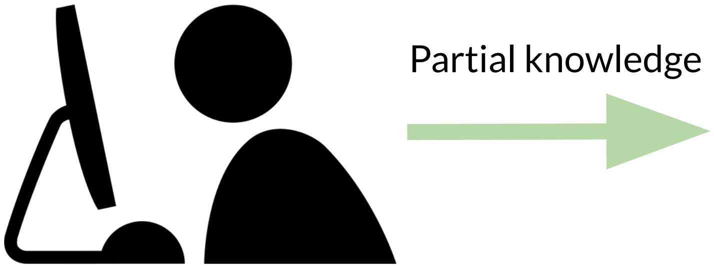
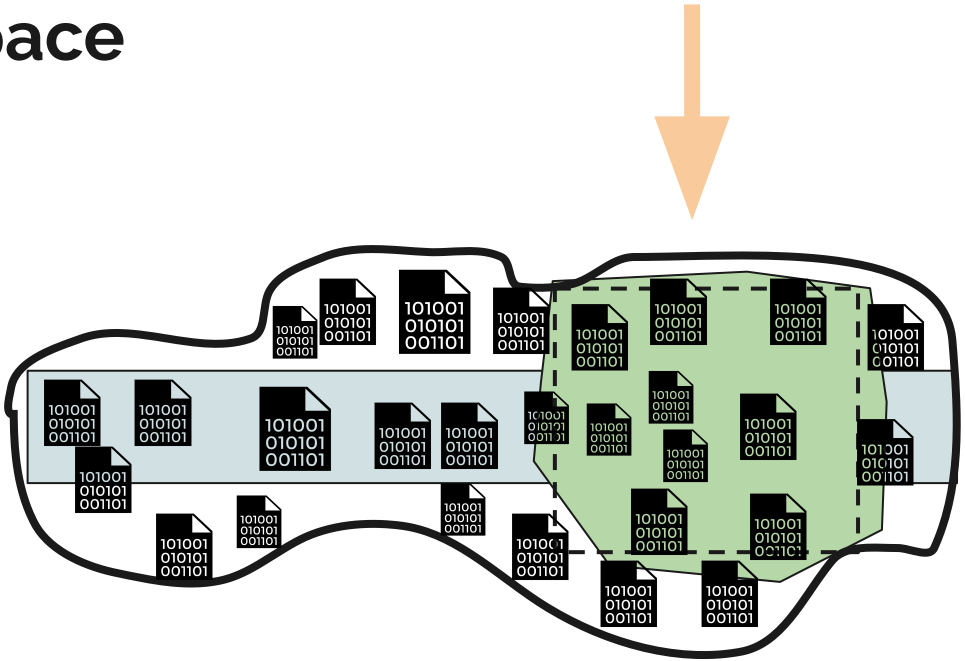


Desirable



{AMS} Workflow

1. User provides a set of API components

2. {AMS} adds alternative API components

3. {AMS} adds complementary API components

4. {AMS} populates the set of hyperparameters and values

5. {AMS} pairs with a user-chosen search procedure, fully defining search space

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Let’s zoom in...

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1. User provides set of API components

Wants linear classifier

Knows LogisticRegression is a linear classifier

```
{
    LogisticRegression
}
```

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2. {AMS} adds alternative API components

Functionally-related components

Insight: Use **component descriptions** to identify **related components**

2. {AMS} uses API documentation

Natural language descriptions

```
In [3]: help(sklearn.linear_model.LogisticRegression)

Help on class LogisticRegression in module sklearn.linear_model._logistic:

class LogisticRegression(sklearn.base.BaseEstimator, sklearn.linear_model._base.Linea
rClassifierMixin, sklearn.linear_model._base.SparseCoefMixin)
 |  LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=
True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_
iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None
)
 |
 |  Logistic Regression (aka logit, MaxEnt) classifier.
 |
 |  In the multiclass case, the training algorithm uses the one-vs-rest (OvR)
 |  scheme if the 'multi_class' option is set to 'ovr', and uses the
```

2. {AMS} adds alternative API components

Use initial **specification documentation as query**

Retrieved components are *relevant* and *related*

2. {AMS} adds alternative API components

D: **document** $\rightarrow$ **potential** components' documentation

Q: **query** $\rightarrow$ **existing** components' documentation

C: **corpus** $\rightarrow$ complete **API documentation**

$$\mathrm{BM25}(D,Q)=\sum_{i}^{n}\mathrm{IDF}(C,q_i)\frac{f(q_i,D)*(k_1+1)}{f(q_i,D)+k_1*\left(1-b+b*\frac{\mathrm{Len}(D)}{\mathrm{AvgLen}(C)}\right)}$$

```
{
    LogisticRegression,
    LinearSVC
}
```

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3. {AMS} adds complementary API components

Complementary Components

Insight: **useful** components appear **together** in **existing code**

3. {AMS} uses existing source code

In [4]:

```
xgb = XGBClassifier(learning_rate=0.02, n_estimators=600, objective='binary:logistic',
                    silent=True, nthread=1)
```

In [14]:

```
from sklearn.preprocessing import MinMaxScaler
mms = MinMaxScaler(feature_range=(0,1))
X_train = mms.fit_transform(X_train)
X_test = mms.fit_transform(X_test)
```

In [15]:

```
svc_classifier.fit(X_train,y_train)
y_pred=svc_classifier.predict(X_test)
```

3. {AMS} uses existing source code

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```

3. {AMS} adds complementary API components

Pointwise Mutual Information: appear **more than expected** if independent?

$$\frac{p(x,y)}{p(x)p(y)}$$

3. {AMS} adds complementary API components

Normalized Pointwise Mutual Information (-1, 1)

Build NPMI-based association rules table

$$\frac{p(x,y)}{p(x)p(y)} \longrightarrow \mathrm{NPMI}(x,y) = \frac{\log_2\left(\frac{p(x,y)}{p(x)p(y)}\right)}{-\log_2(p(x,y))}$$

```
{
    PolyFeatures,
    MinMaxScaler,
    VarianceThreshold,
    LogisticRegression,
    LinearSVC
}
```

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4. {AMS} populates hyperparameters

Different algorithms have different hyperparameters to choose/tune

Insight: users’ code sets/tunes **useful** hyperparameters

4. {AMS} uses existing source code

In [4]:

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In [15]:

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y_pred=svc_classifier.predict(X_test)
```

4. {AMS} populates hyperparameters

Just **count**!

Top-k frequency distribution

```
{
    PolyFeatures: {"degree":[2, 3, 4]},
    MinMaxScaler: {},
    VarianceThreshold: {"threshold": [0.2]},
    LogisticRegression: {
        "penalty":["l1", "elastic"], "C": [0.1, 100.0],
    },
    LinearSVC: {
        "penalty":["l1"], "C": [0.1],
    }
}
```

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5. {AMS} pairs with different sampling approaches

Genetic Programming (TPOT)

Random search

Performance Evaluation

Concept of Pipeline Win

- Start with N systems
- Pick best pipeline from each one (F1 score on held-out test set)
- Compare all best pipelines
- System K wins if
  - It has best pipeline and
  - Its pipeline has F1 score at least 0.01 larger than next closest pipeline

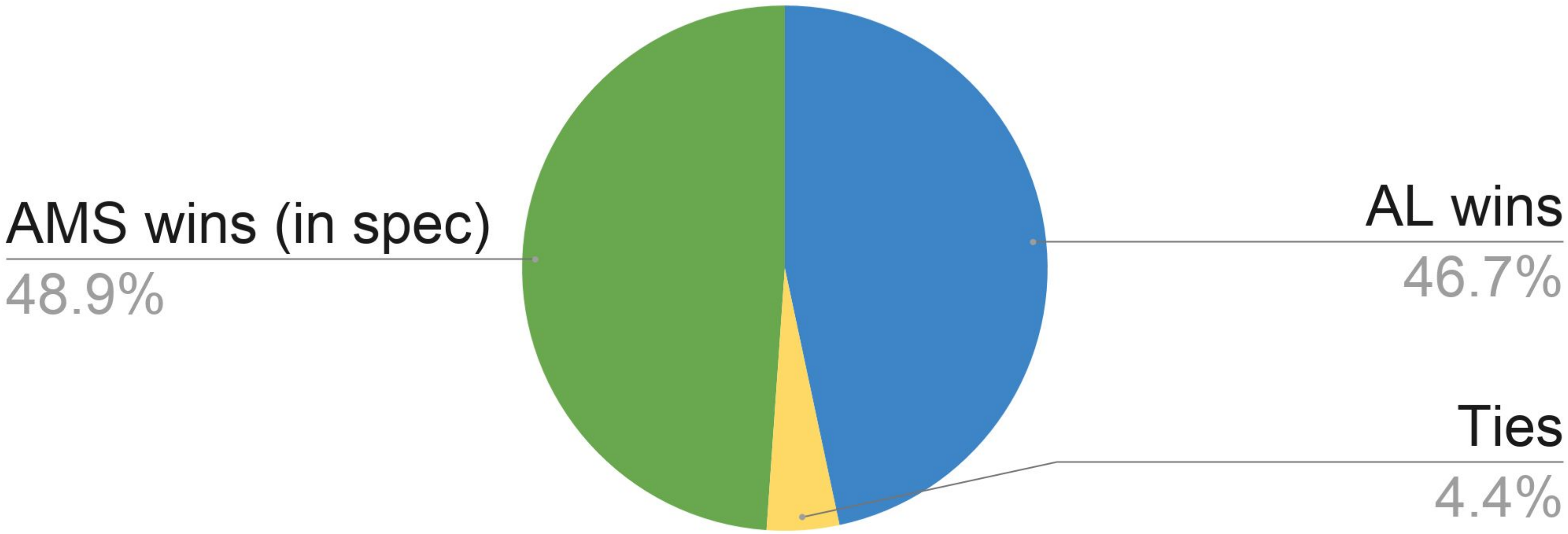
Comparison with AL

- AL: AutoML tool that learns from existing code (OOPSLA 2019)
- AL gives **limited control** over **pipelines produced**
  - Like existing AutoML tools
- **AMS exposes control** through weak specifications and their augmentation

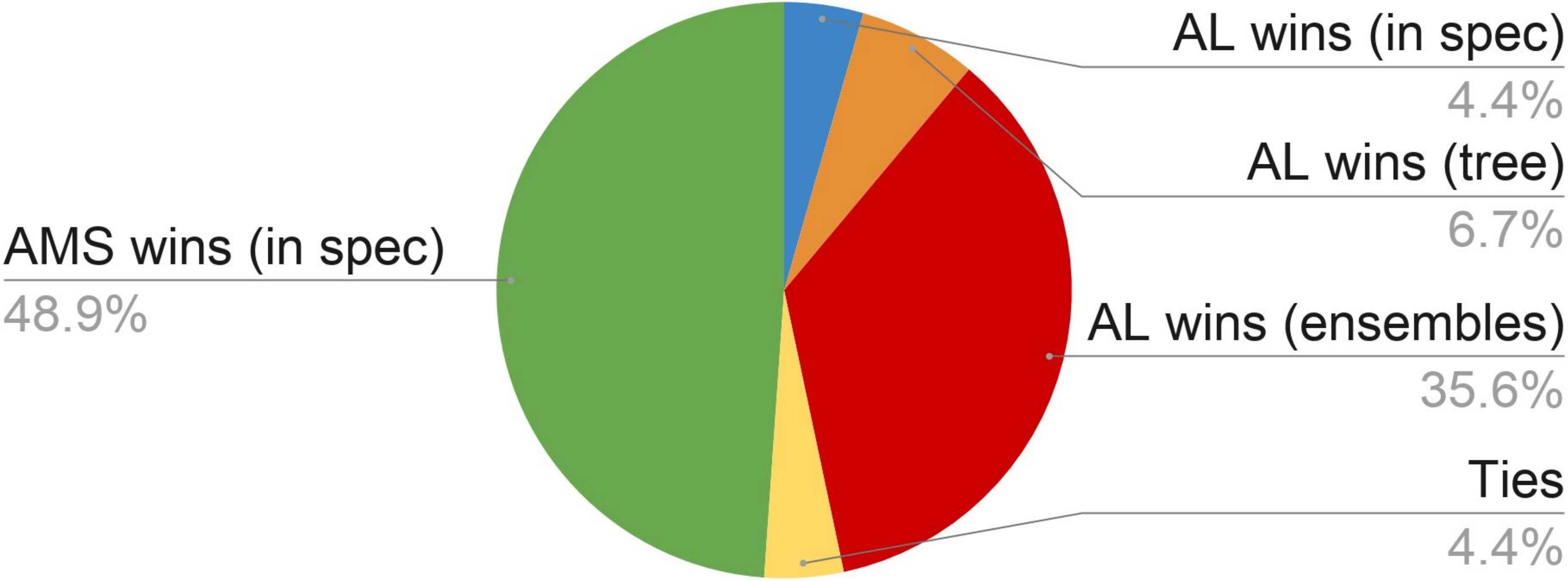
Comparison with AL

- 9 datasets, 5-fold cross validation
- Total 45 pipelines generated by each system
- Specification:

{LogisticRegression, LinearSVC, StandardScaler}


AMS wins (in spec)
48.9%
AL wins
46.7%
Ties
4.4%

...but AL doesn't use spec

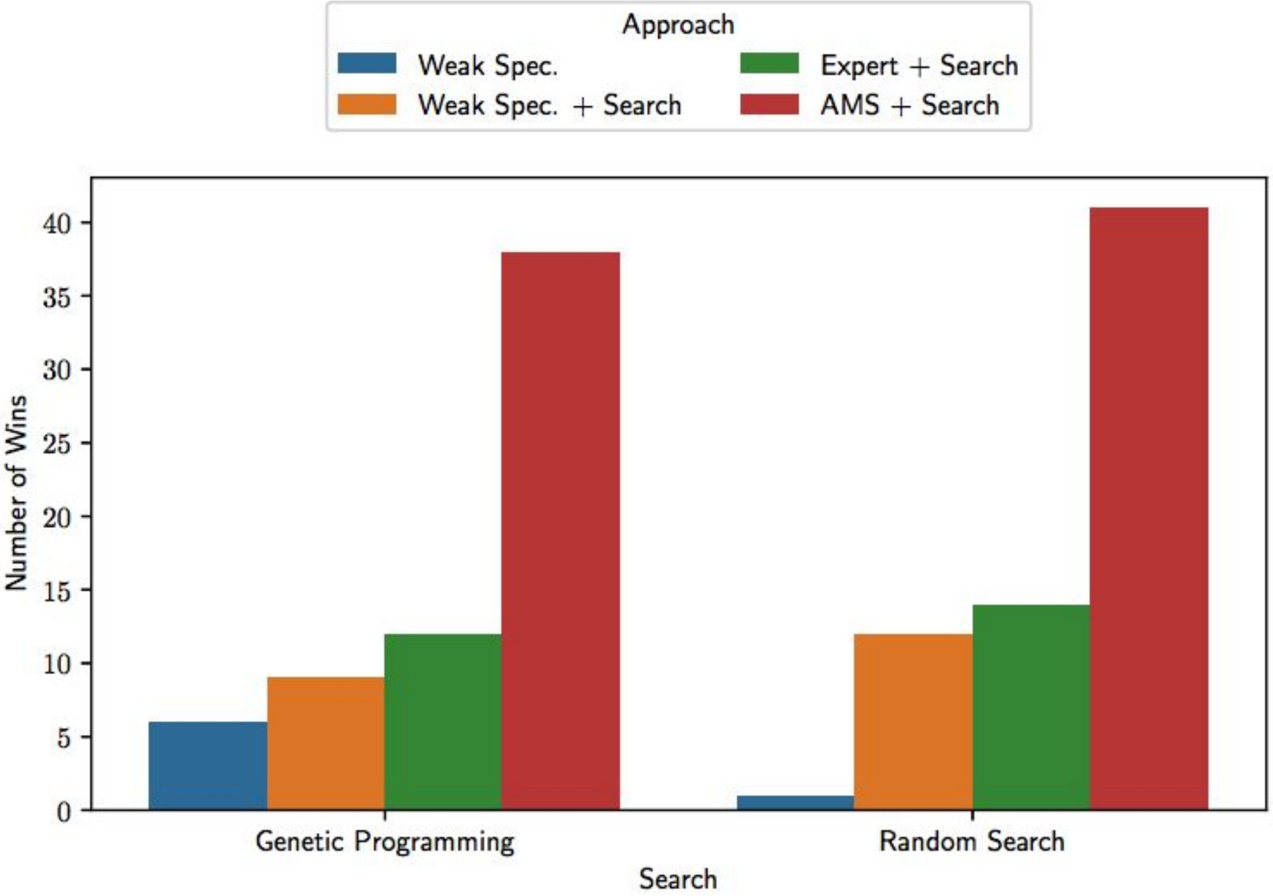


… AMS does

- All pipelines produced adhere to spec
- 42 wins after removing non-spec adherent AL pipelines

More Performance Evaluation

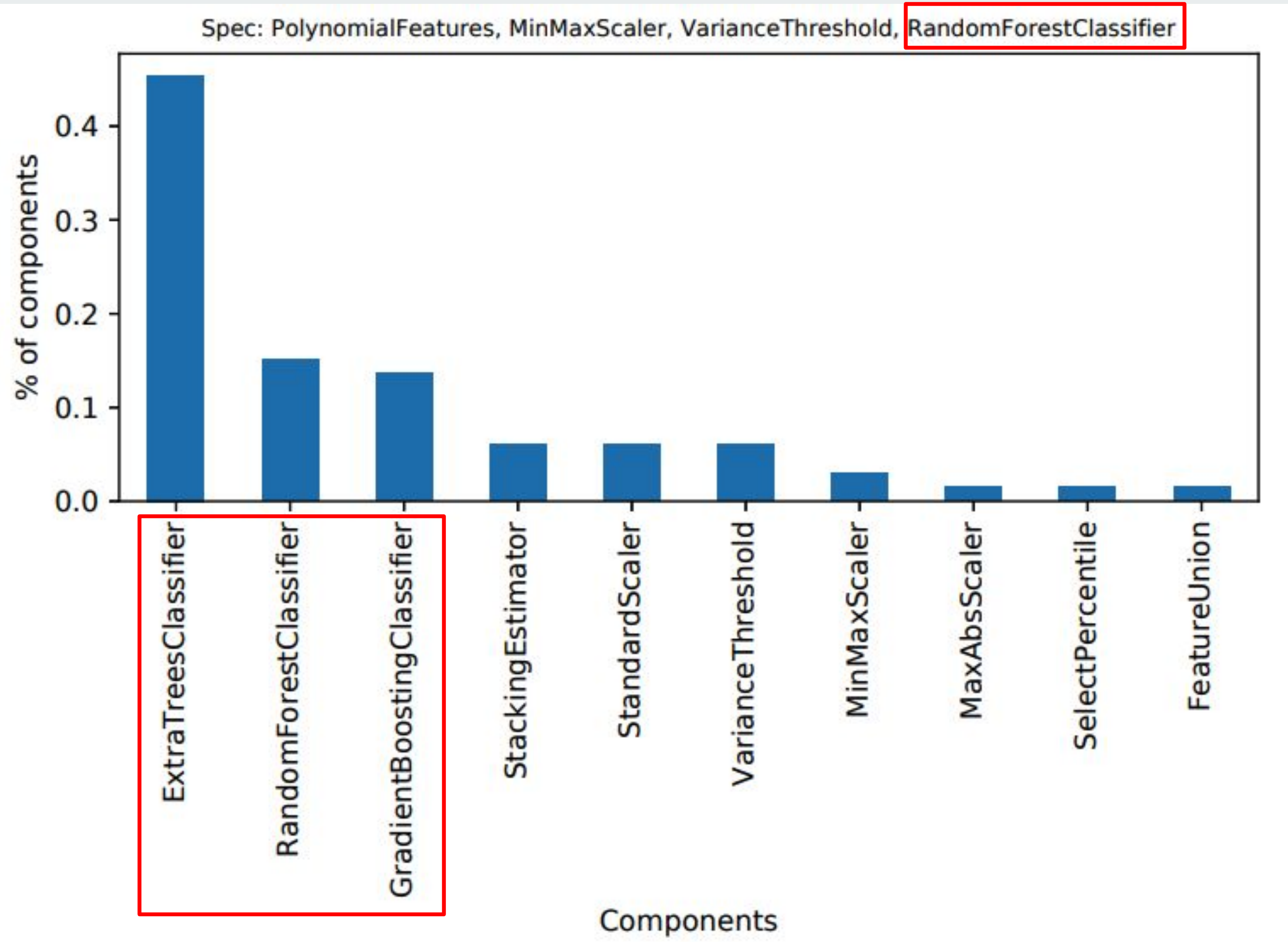
- Comparisons
  - Weak spec as pipeline
  - Weak spec + Search
  - Expert hyperparameters/values for weak spec + Search
  - AMS + Search
- Generate 15 weak specifications by composing popular components
  - 3 classifiers (logistic regression, random forest, decision tree)
  - 4 preprocessors (feature scaling, polynomial features, PCA, variance-based feature selection)
- 5 minutes search budget, 9 datasets
- 5-fold cross-validation

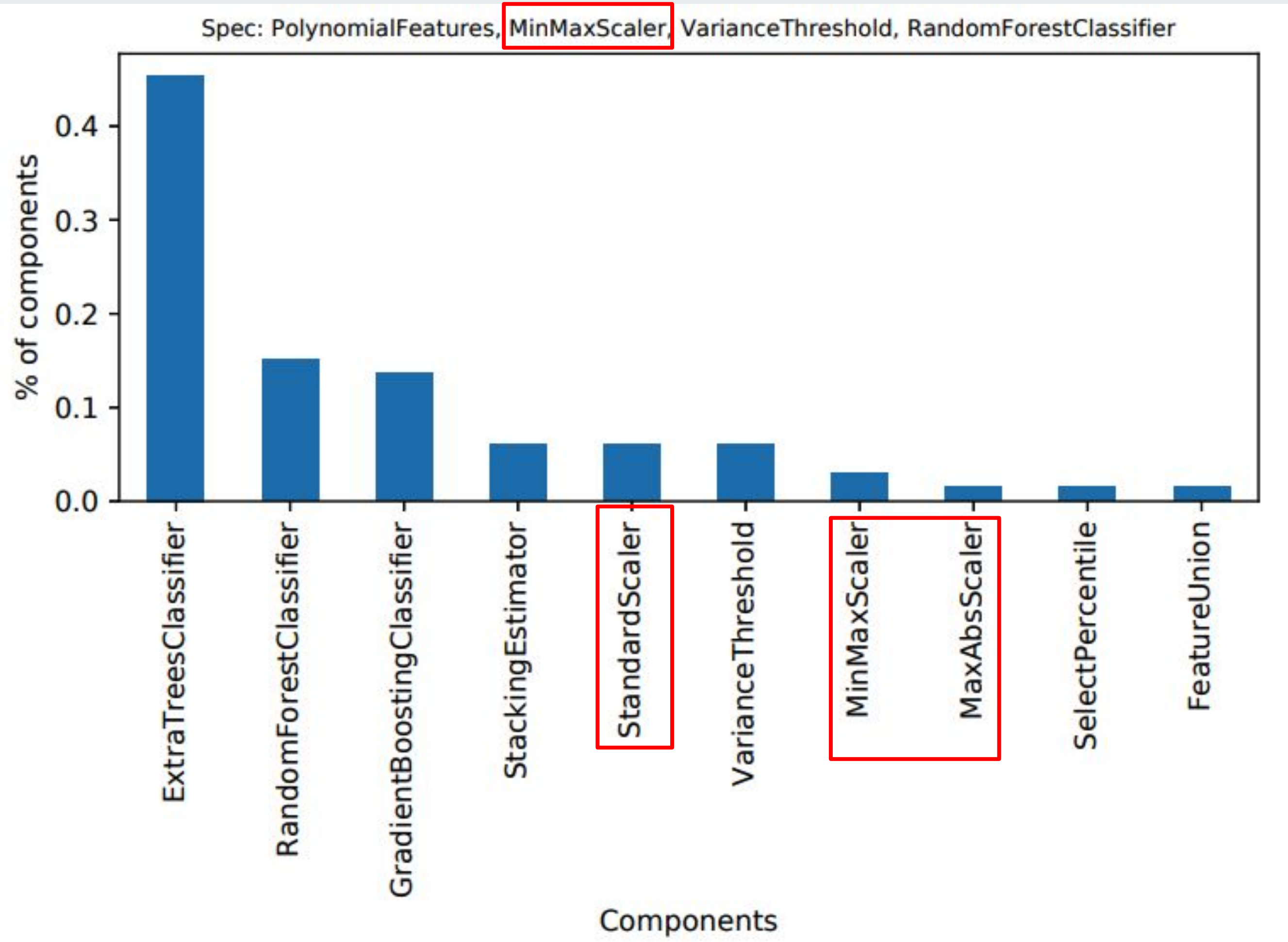


Approach
Weak Spec.
Weak Spec. + Search
Expert + Search
AMS + Search
Number of Wins
0
5
10
15
20
25
30
35
40
Genetic Programming
Random Search
Search

And pipelines generated reflect spec...

```
{
    PolynomialFeatures,
    MinMaxScaler,
    VarianceThreshold,
    RandomForestClassifier,
}
```


Spec: PolynomialFeatures, MinMaxScaler, VarianceThreshold, RandomForestClassifier
% of components
0.0
0.1
0.2
0.3
0.4
ExtraTreesClassifier
RandomForestClassifier
GradientBoostingClassifier
StackingEstimator
StandardScaler
VarianceThreshold
MinMaxScaler
MaxAbsScaler
SelectPercentile
FeatureUnion
Components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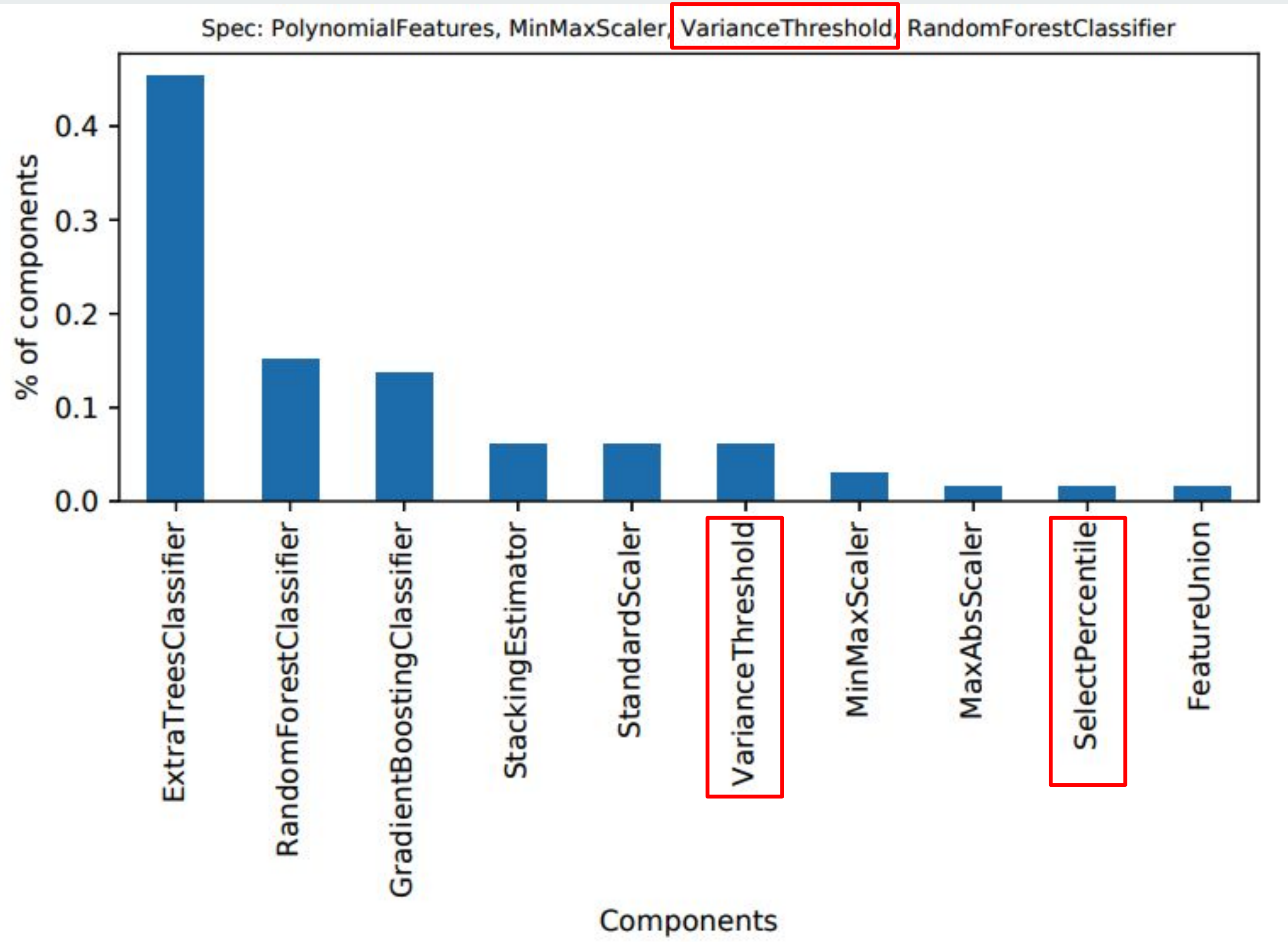
Spec: PolynomialFeatures, MinMaxScaler, VarianceThreshold, RandomForestClassifier
% of components
0.4
0.3
0.2
0.1
0.0
ExtraTreesClassifier
RandomForestClassifier
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Additional results in paper

- Precision for functionally related component retrieval
- Precision for complementary component rules
- Characterize hyperparameter use in corpus
- Impact of varying corpus size
- And more!

AMS: A new model for interacting with AutoML

Partial user information (Weak Specification)	Automated Augmentation

- Automatically generate search space
- Reflect influence of original specification

Additional Information

- Paper
- Zenodo Artifact
- Github

Image Courtesy

- Binary Icon: Creative Stall (Noun Project)
- User Icon: Luis Prado (Noun Project)