Type-Driven Automated Learning with LALE

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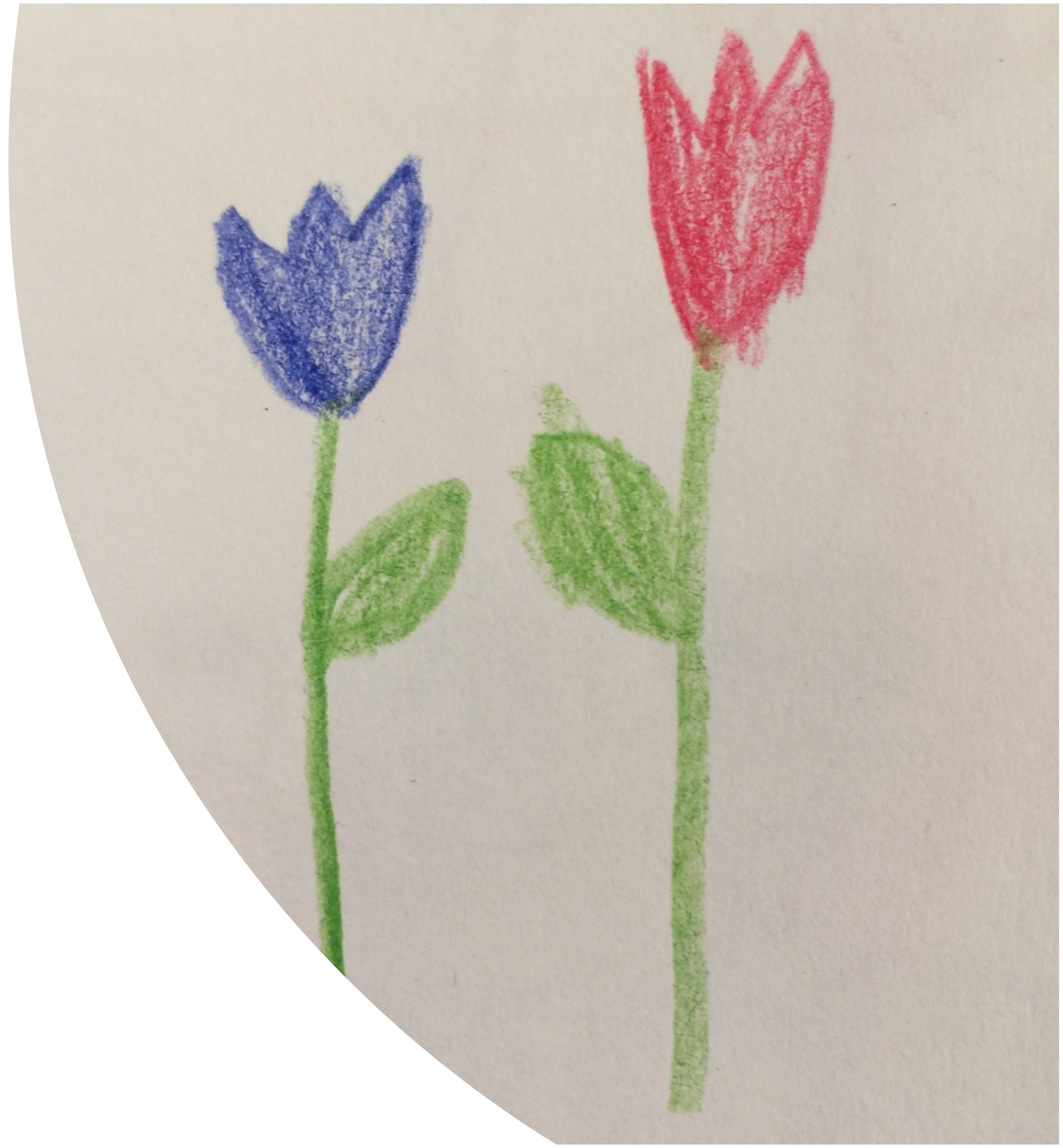
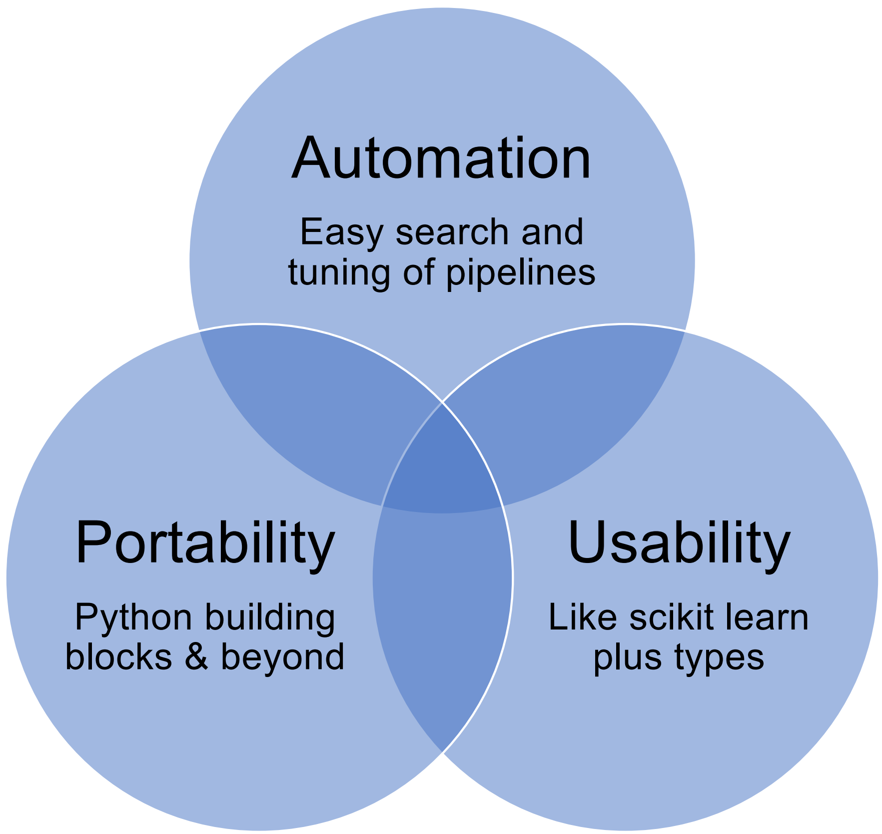


Value Proposition

Augment, but don't replace, the data scientist.



Manual ML with Sklearn

Prior work: scikit learn, popular machine learning package

```
pca_lr = make_pipeline(PCA(svd_solver='full', n_components=0.3),
                       LR(solver='liblinear', penalty='l1'))
```

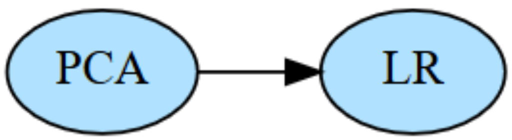
```
pca_lr.fit(train_X, train_y)
predicted = pca_lr.predict(test_X)
print(f'accuracy  {accuracy_score(test_y, predicted):.1%}')
```

```
accuracy  70.2%
```

Manual ML with LALE

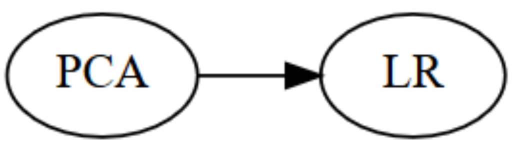
Our work: Language for Automated Learning Exploration

```
pca_lr = PCA(PCA.svd_solver.full, n_components=0.3) \
      >> LR(LR.solver.liblinear, LR.penalty.l1)
to_graphviz(pca_lr)
```




```
trained = pca_lr.fit(train_X, train_y)
predicted = trained.predict(test_X)
print(f'accuracy  {accuracy_score(test_y, predicted):.1%}')
to_graphviz(trained)
```

```
accuracy  70.2%
```



LALE Pipelines

- Pipeline Combinators:

LALE features	Name	Description	Scikit-learn features
`>>` `make_pipeline`	pipe	feed to next	`make_pipeline`
`&` `make_union`	and	run both	`make_union` or `ColumnTransformer`
`|` `make_choice`	or	choose one	N/A (specific to given AI automation tool)

- Example:

```
((PCA & MinMaxScaler)
 >> Concat
 >> (KNN | DecisionTree))
```

Constraints in Manual ML

Conditional hyperparameters

```
pca_lr = make_pipeline(PCA(svd_solver='full', n_components=0.3),
                       LR(solver='sag', penalty='l1'))
```

```
pca_lr.fit(train_X, train_y)
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-7-de82d92d1962> in <module>
----> 1 pca_lr.fit(train_X, train_y)

~/python3.7venv/lib/python3.7/site-packages/sklearn/pipeline.py in fit(self, X, y, **fit_params)
    265         Xt, fit_params = self._fit(X, y, **fit_params)
    266         if self._final_estimator is not None:
--> 267             self._final_estimator.fit(Xt, y, **fit_params)
    268         return self
    269 

~/python3.7venv/lib/python3.7/site-packages/sklearn/linear_model/logistic.py in fit(self, X, y, sample_weight)
   1275                              "positive; got (tol=%r)" % self.tol)
   1276 
-> 1277         solver = _check_solver(self.solver, self.penalty, self.dual)
   1278 
   1279         if solver in ['newton-cg']:

~/python3.7venv/lib/python3.7/site-packages/sklearn/linear_model/logistic.py in _check_solver(solver, penalty, dual)
    445     if solver not in ['liblinear', 'saga'] and penalty != 'l2':
    446         raise ValueError("Solver %s supports only l2 penalties, "
--> 447                          "got %s penalty." % (solver, penalty))
    448     if solver != 'liblinear' and dual:
    449         raise ValueError("Solver %s supports only "

ValueError: Solver sag supports only l2 penalties, got l1 penalty.
```

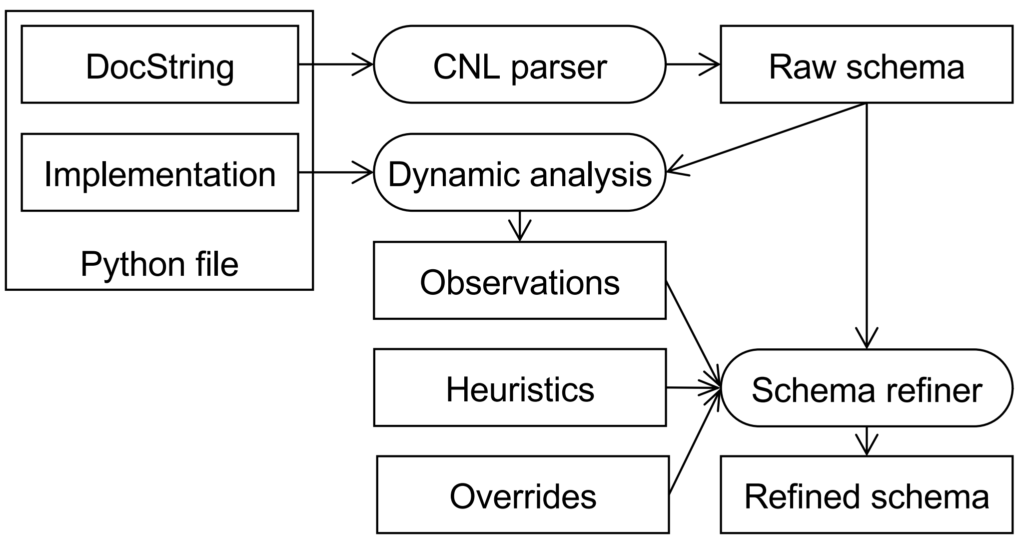
(JSON) Schemas for ML Algorithms

- Use of JSON schema for defining hyper-parameter types and search spaces, input and output types.
- Example hyper-parameter schema for LogisticRegression:

```
LR: { allOf: [
  { type: object,
    properties: {
      S: { description: "Optimization problem solver",
           enum: [linear, sag, lbfgs], default: linear},
      P: { description: "Penalization norm",
           enum: [l1, l2], default: l2}}},
  { description: "Solvers sag and lbfgs support only l2.",
    anyOf: [
      { not: { type: object, properties: {S: {enum: [sag, lbfgs]}}}},
      { type: object, properties: {P: {enum: [l2]}}}]}]}
```

Most users do not need to write these schemas. Usually, the operator writer adds these once and uses them multiple times for multiple purposes.

Automated Schema Extractor



https://github.com/IBM/lale/tree/master/lale/lib/autogen

Customizing Schemas by Hand

```
from lale.schemas import Null, Enum, Int, Float, Object, Array, Not, AnyOf

MyLR = MyLR.customize_schema(
    relevantToOptimizer=['solver', 'penalty', 'C'],
    solver=Enum(desc='Algorithm for optimization problem.',
                values=['newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'],
                default='liblinear'),
    penalty=Enum(desc='Norm used in the penalization.',
                 values=['l1', 'l2'],
                 default='l2'),
    C=Float(desc='Inverse regularization strength. '
                 'Smaller values specify stronger regularization.',
            min=0.0, exclusiveMin=True,
            minForOptimizer=0.03125, maxForOptimizer=32768,
            distribution='loguniform',
            default=1.0))
```

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/docs_new_operators_schemas_api.ipynb

Constraints in LALE

In [16]:

```
%%time
import jsonschema
try:
    lale_misconfigured = Tfidf >> LR(LR.solver.sag, LR.penalty.l1)
except jsonschema.ValidationError as e:
    print(e.message, file=sys.stderr)
```

```
CPU times: user 46.9 ms, sys: 15.6 ms, total: 62.5 ms
Wall time: 36.7 ms
```

```
Invalid configuration for LR(solver='sag', penalty='l1') due to constraint the newton-cg, s
ag, and lbfgs solvers support only l2 penalties.
Schema of constraint 1: {
    'description': 'The newton-cg, sag, and lbfgs solvers support only l2 penalties.',
    'anyOf': [{
        'type': 'object',
        'properties': {
            'solver': {
                'not': {
                    'enum': ['newton-cg', 'sag', 'lbfgs']}}}}, {
        'type': 'object',
        'properties': {
            'penalty': {
                'enum': ['l2']}}}],
}
Value: {'solver': 'sag', 'penalty': 'l1', 'dual': False, 'C': 1.0, 'tol': 0.0001, 'fit_inte
rcept': True, 'intercept_scaling': 1.0, 'class_weight': None, 'random_state': None, 'max_it
er': 100, 'multi_class': 'ovr', 'verbose': 0, 'warm_start': False, 'n_jobs': None}
```

AutoML (GridSearchCV)

Create Hyperparameter Search Space

```
# Create regularization penalty space
penalty = ['l1', 'l2']

# Create regularization hyperparameter space
C = np.logspace(0, 4, 10)

# Create hyperparameter options
hyperparameters = dict(C=C, penalty=penalty)
```

Create Grid Search

```
# Create grid search using 5-fold cross validation
clf = GridSearchCV(logistic, hyperparameters, cv=5, verbose=0)
```

Constraints in AutoML

Problem: Some automated iterations raise exceptions

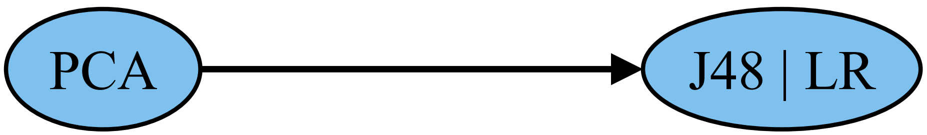
Solution 1: Unconstrained search space

- $\{S{:}[\mathit{linear},\mathit{sag},\mathit{lbfgs}],\ P{:}\ [\mathit{l1},\mathit{l2}]\}$
- Catch exception
- Return made-up loss `np.float.max`

Solution 2: Constrained search space

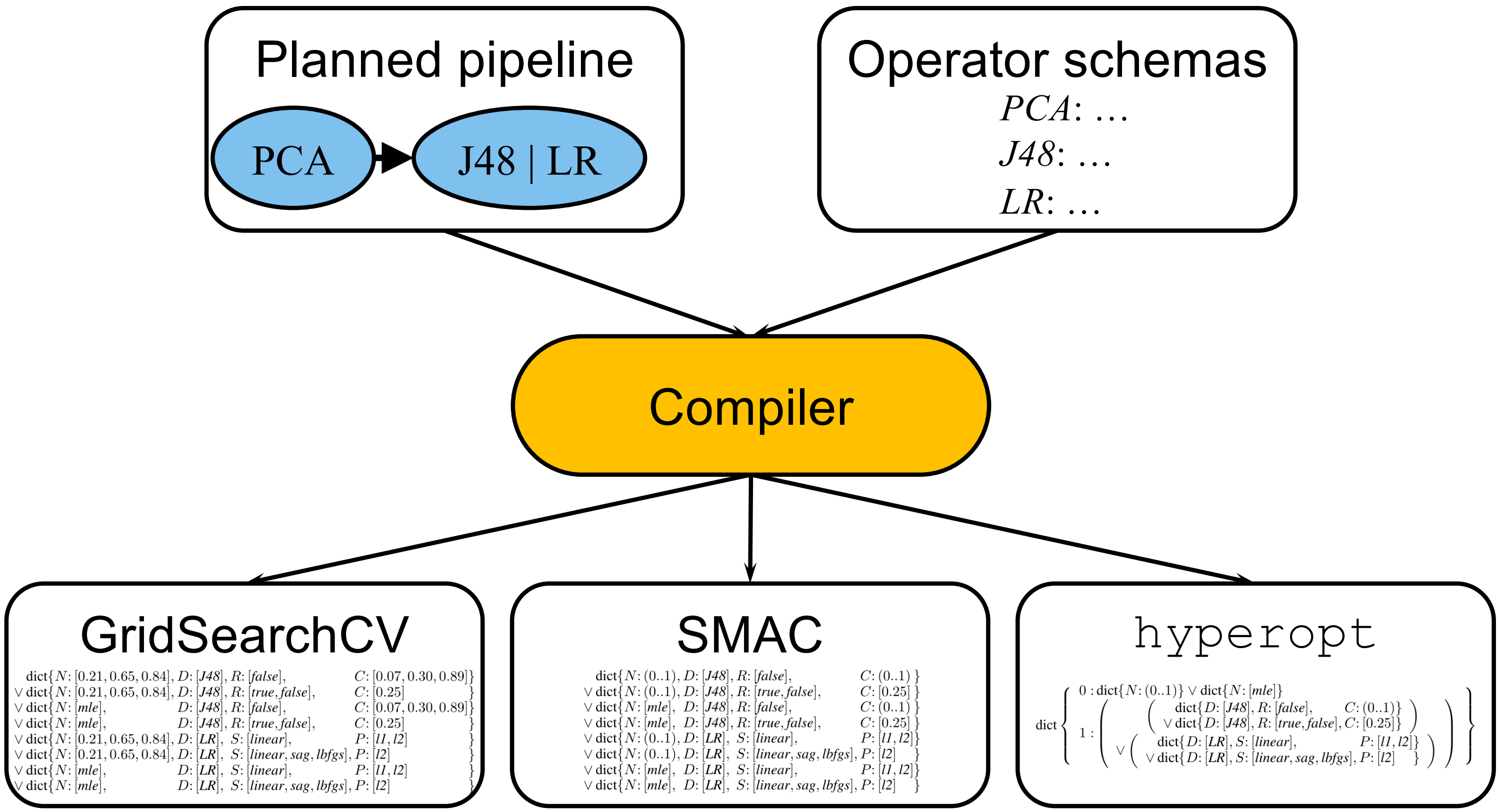
- $\{S{:}[\mathit{linear},\mathit{sag},\mathit{lbfgs}],\ P{:}\ [\mathit{l1},\mathit{l2}]\}$ **and** (**if** S: $[\mathit{sag},\mathit{lbfgs}]$ **then** P: $[\mathit{l2}]$)
- No exceptions
- No made-up loss

Algorithm Selection



Types as Search Spaces

LALE auto-generates search spaces for AutoML tools



GridSearchCV Search Space

AutoML included with Sklearn

$$
\begin{array}{lllll}
 & \text{dict}\{N\colon [0.21, 0.65, 0.84], & D\colon [\mathit{J48}], R\colon [\mathit{false}], & C\colon [0.07, 0.30, 0.89] & \} \\
\vee & \text{dict}\{N\colon [0.21, 0.65, 0.84], & D\colon [\mathit{J48}], R\colon [\mathit{true}, \mathit{false}], & C\colon [0.25] & \} \\
\vee & \text{dict}\{N\colon [\mathit{mle}], & D\colon [\mathit{J48}], R\colon [\mathit{false}], & C\colon [0.07, 0.30, 0.89] & \} \\
\vee & \text{dict}\{N\colon [\mathit{mle}], & D\colon [\mathit{J48}], R\colon [\mathit{true}, \mathit{false}], & C\colon [0.25] & \} \\
\vee & \text{dict}\{N\colon [0.21, 0.65, 0.84], & D\colon [\mathit{LR}], \ S\colon [\mathit{linear}], & P\colon [\mathit{l1}, \mathit{l2}] & \} \\
\vee & \text{dict}\{N\colon [0.21, 0.65, 0.84], & D\colon [\mathit{LR}], \ S\colon [\mathit{linear}, \mathit{sag}, \mathit{lbfgs}], & P\colon [\mathit{l2}] & \} \\
\vee & \text{dict}\{N\colon [\mathit{mle}], & D\colon [\mathit{LR}], \ S\colon [\mathit{linear}], & P\colon [\mathit{l1}, \mathit{l2}] & \} \\
\vee & \text{dict}\{N\colon [\mathit{mle}], & D\colon [\mathit{LR}], \ S\colon [\mathit{linear}, \mathit{sag}, \mathit{lbfgs}], & P\colon [\mathit{l2}] & \}
\end{array}
$$

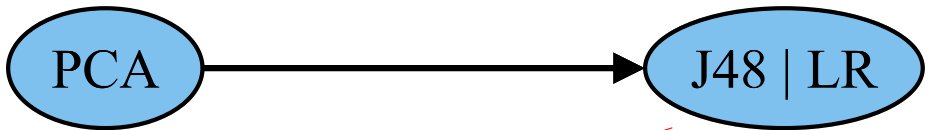
SMAC Search Space

Sequential Model-based Algorithm Configuration

$$
\begin{aligned}
& \text{dict}\{N\colon (0..1), D\colon [\mathit{J48}], R\colon [\mathit{false}], && C\colon (0..1)\ \} \\
\vee\ & \text{dict}\{N\colon (0..1), D\colon [\mathit{J48}], R\colon [\mathit{true}, \mathit{false}], && C\colon [0.25]\ \} \\
\vee\ & \text{dict}\{N\colon [\mathit{mle}],\ D\colon [\mathit{J48}], R\colon [\mathit{false}], && C\colon (0..1)\ \} \\
\vee\ & \text{dict}\{N\colon [\mathit{mle}],\ D\colon [\mathit{J48}], R\colon [\mathit{true}, \mathit{false}], && C\colon [0.25]\ \} \\
\vee\ & \text{dict}\{N\colon (0..1), D\colon [\mathit{LR}],\ S\colon [\mathit{linear}], && P\colon [\mathit{l1}, \mathit{l2}]\} \\
\vee\ & \text{dict}\{N\colon (0..1), D\colon [\mathit{LR}],\ S\colon [\mathit{linear}, \mathit{sag}, \mathit{lbfgs}], && P\colon [\mathit{l2}]\ \} \\
\vee\ & \text{dict}\{N\colon [\mathit{mle}],\ D\colon [\mathit{LR}],\ S\colon [\mathit{linear}], && P\colon [\mathit{l1}, \mathit{l2}]\} \\
\vee\ & \text{dict}\{N\colon [\mathit{mle}],\ D\colon [\mathit{LR}],\ S\colon [\mathit{linear}, \mathit{sag}, \mathit{lbfgs}], && P\colon [\mathit{l2}]\ \}
\end{aligned}
$$

Hyperopt Search Space

Supports parallel search

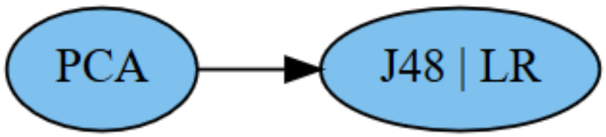


$$\mathrm{dict}\left\{ \begin{array}{l} 0 : \mathrm{dict}\{N\colon (0..1)\} \vee \mathrm{dict}\{N\colon [\mathit{mle}]\} \\ 1 : \left(\begin{array}{l} \left(\begin{array}{l} \quad \mathrm{dict}\{D\colon [\mathit{J48}], R\colon [\mathit{false}], \quad C\colon (0..1)\} \\ \vee \mathrm{dict}\{D\colon [\mathit{J48}], R\colon [\mathit{true}, \mathit{false}], C\colon [0.25]\} \end{array} \right) \\ \vee \left(\begin{array}{l} \quad \mathrm{dict}\{D\colon [\mathit{LR}], S\colon [\mathit{linear}], \quad P\colon [\mathit{l1}, \mathit{l2}]\} \\ \vee \mathrm{dict}\{D\colon [\mathit{LR}], S\colon [\mathit{linear}, \mathit{sag}, \mathit{lbfgs}], P\colon [\mathit{l2}]\} \end{array} \right) \end{array} \right) \end{array} \right\}$$

Automated ML with LALE

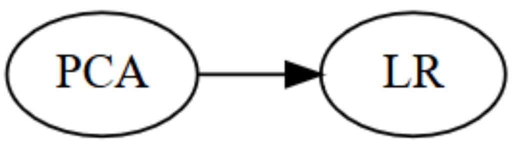
Combined algorithm selection and hyperparameter tuning

```
planned = PCA >> (J48 | LR)
to_graphviz(planned)
```




```
hyperopt_classifier = HyperoptClassifier(planned, max_evals=5)
best_found = hyperopt_classifier.fit(train_X, train_y)
predicted = best_found.predict(test_X)
print(f'accuracy  {accuracy_score(test_y, predicted):.1%}')
to_graphviz(best_found)
```

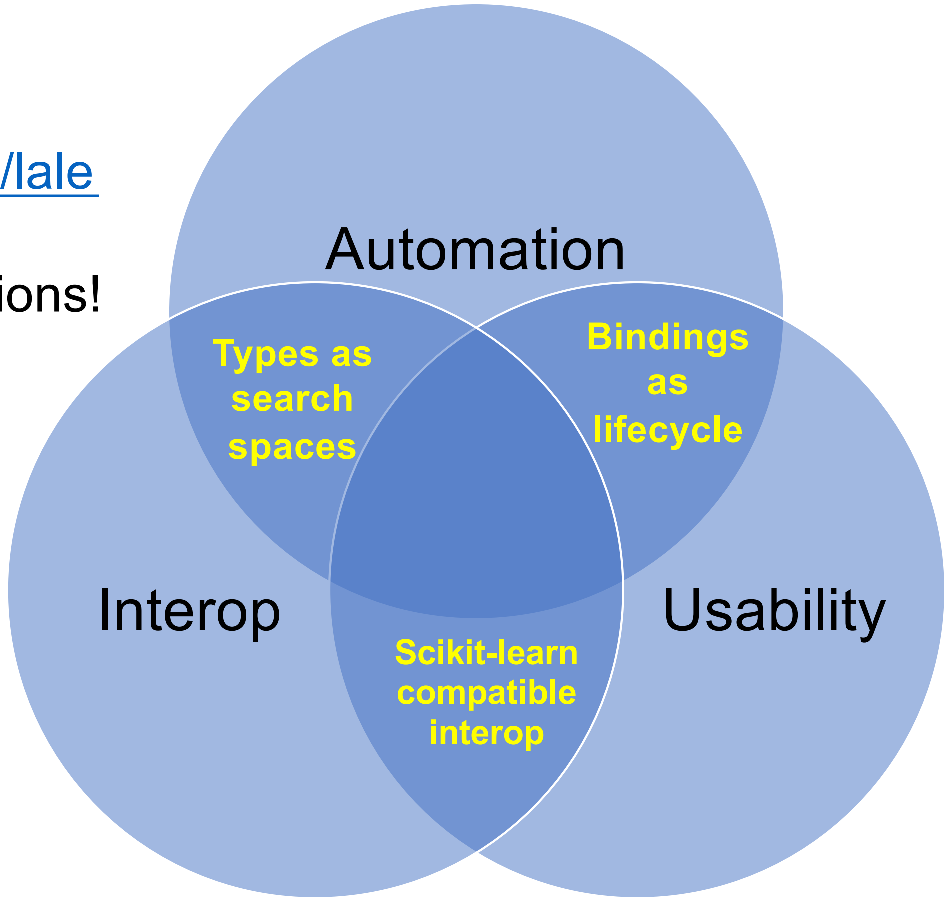
```
accuracy  96.4%
```



Summary

Github URL:
https://github.com/IBM/lale

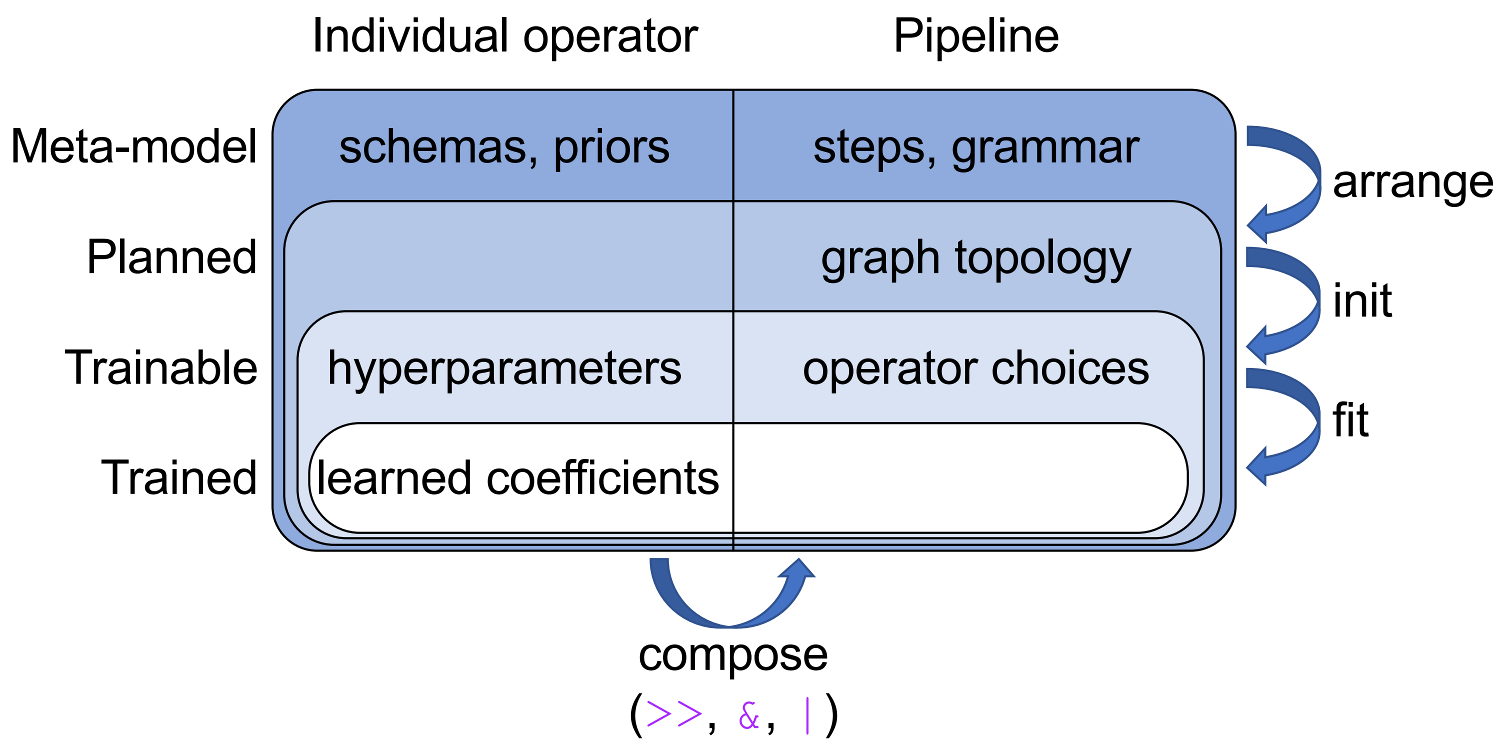
We welcome contributions!



Portability

Modality	Dataset	Pipeline (**bold**: best found choice)
Text	Movie reviews (sentiment analysis)	`(`**`BERT`**` | TFIDF)` `>> (`**`LR`**` | MLP | KNN | SVC | PAC)`
Table	Car (structured with categorical features)	**`J48`**`	ArulesCBA	LR	KNN`
Images	CIFAR-10 (image classification)	**`ResNet50`**
Time-series	Epilepsy (seizure classification)	**`WindowTransformer`** `>> (`**`KNN`**` | XGBoost | LR)` `>> `**`Voting`**

Bindings as Lifecycle



Summary

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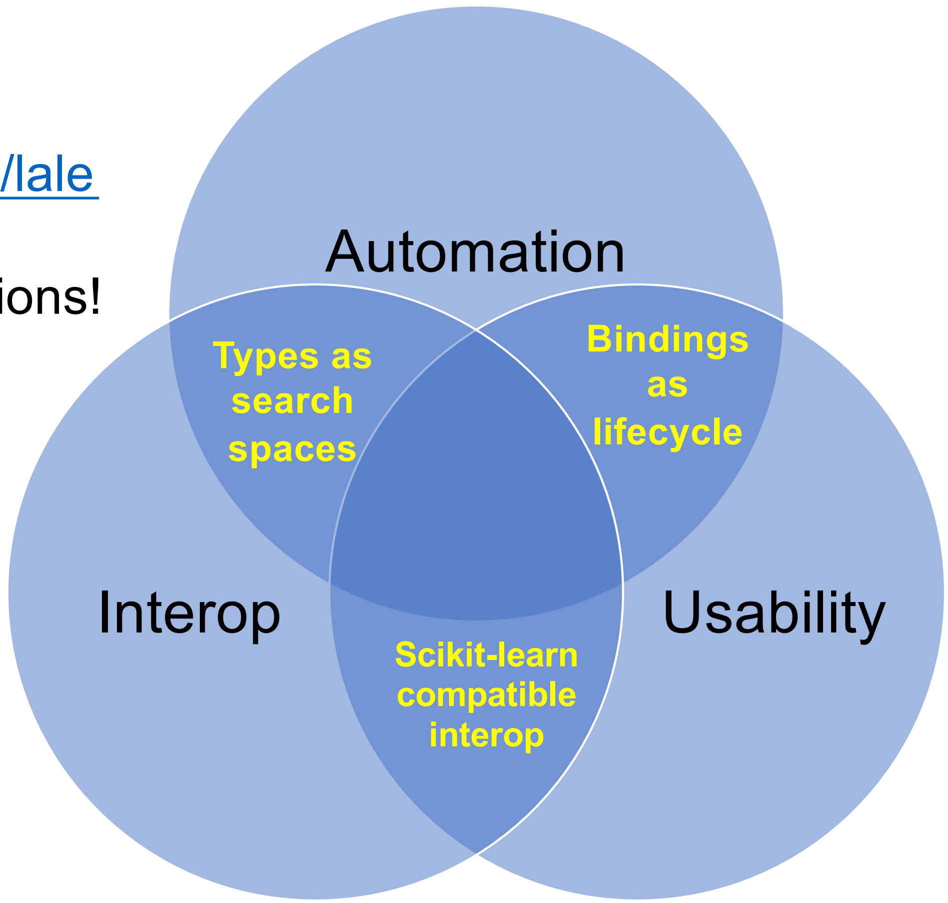
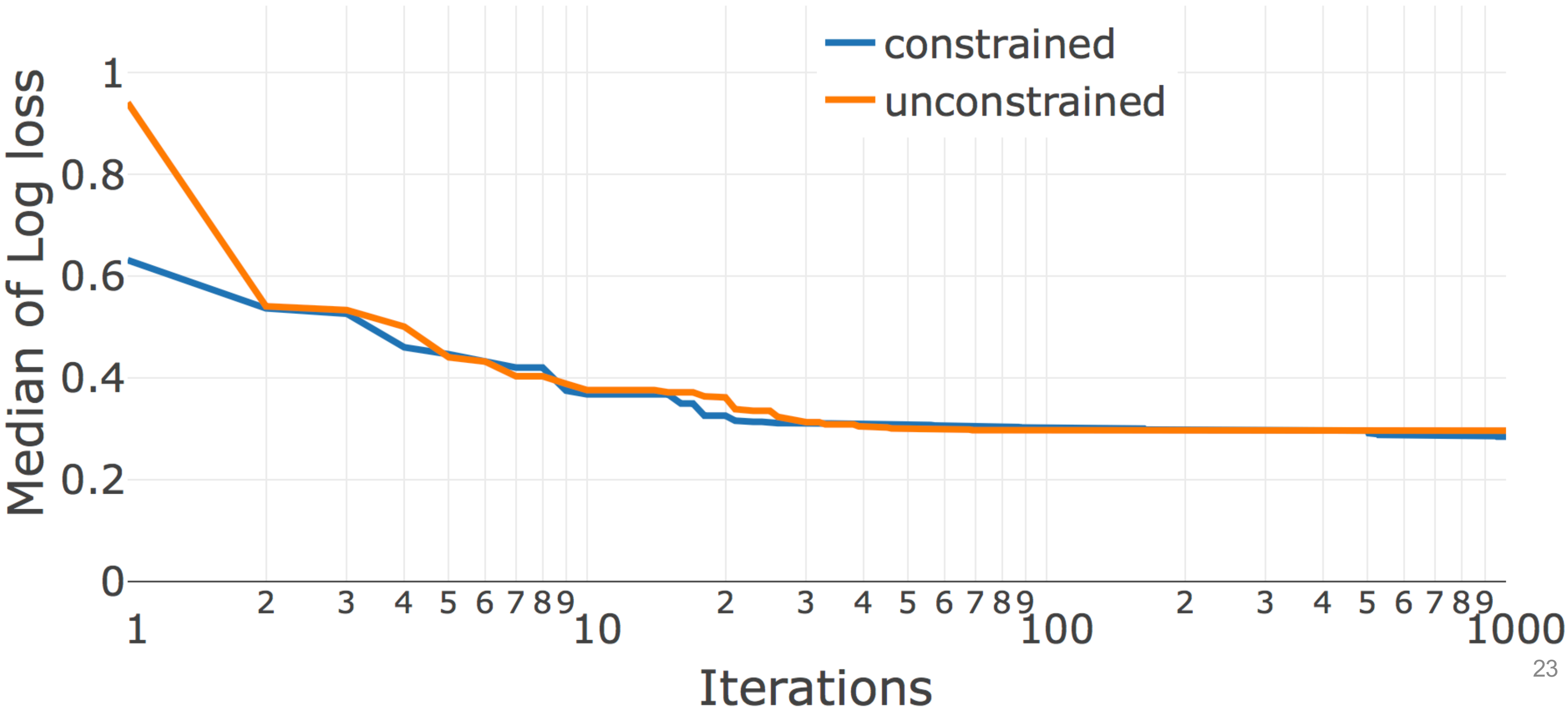


Search Convergence (1/3)

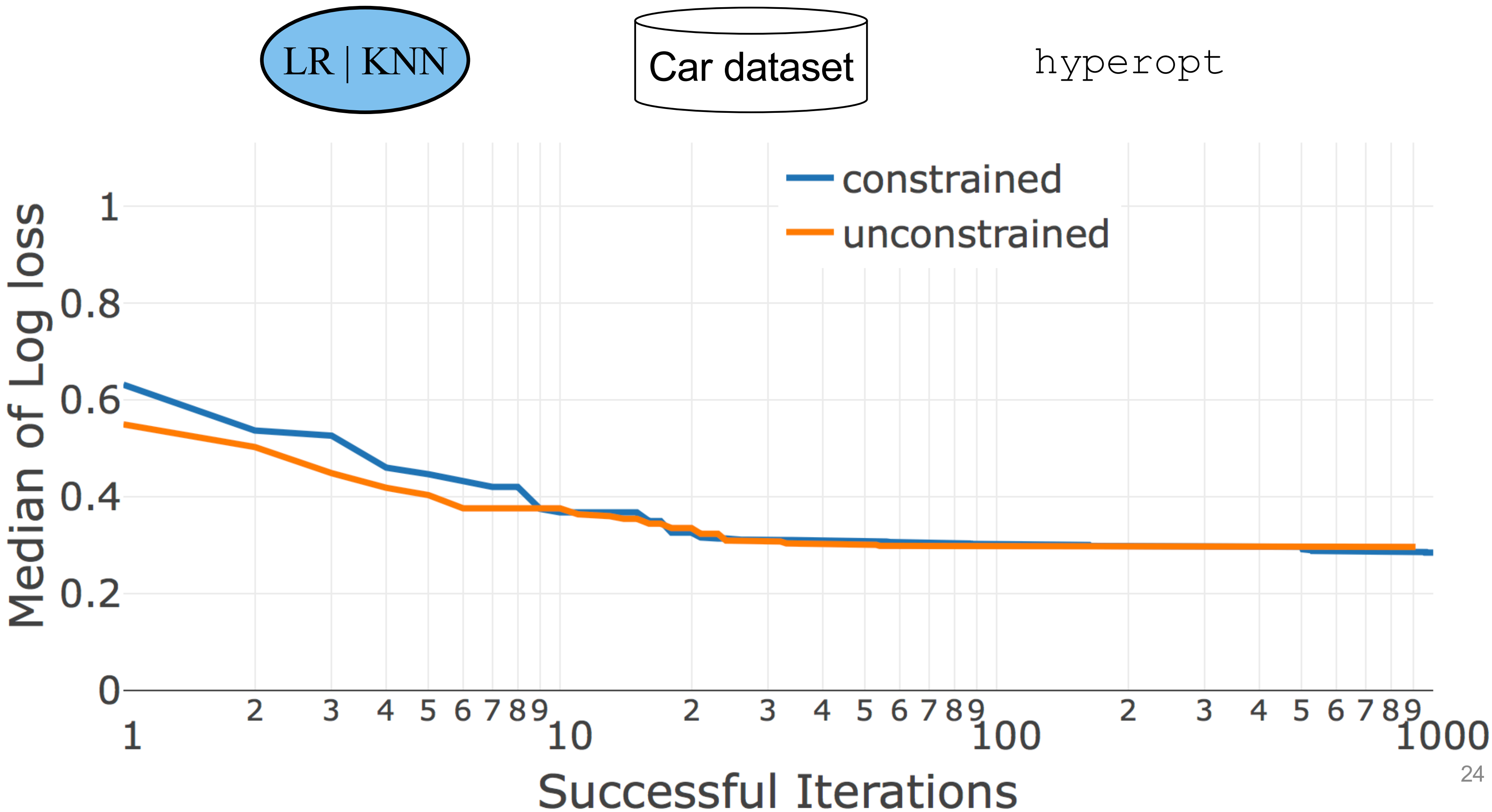
LR | KNN

Car dataset

hyperopt



Search Convergence (2/3)



Search Convergence (3/3)

J48 | LR | KNN

Car dataset

hyperopt