Type-Driven Automated Learning with LALE

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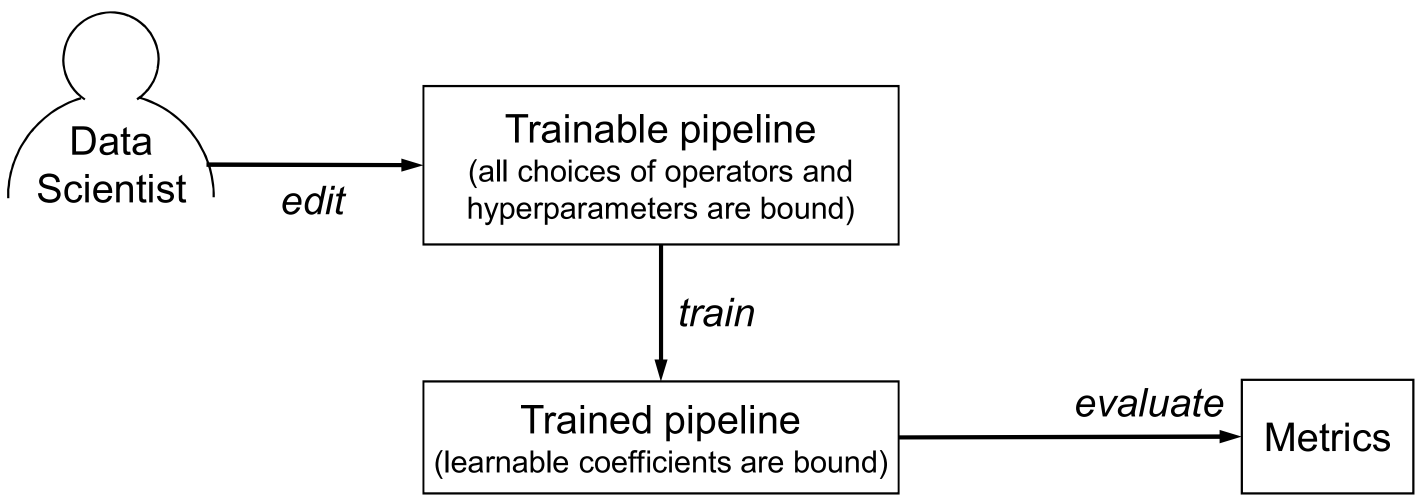
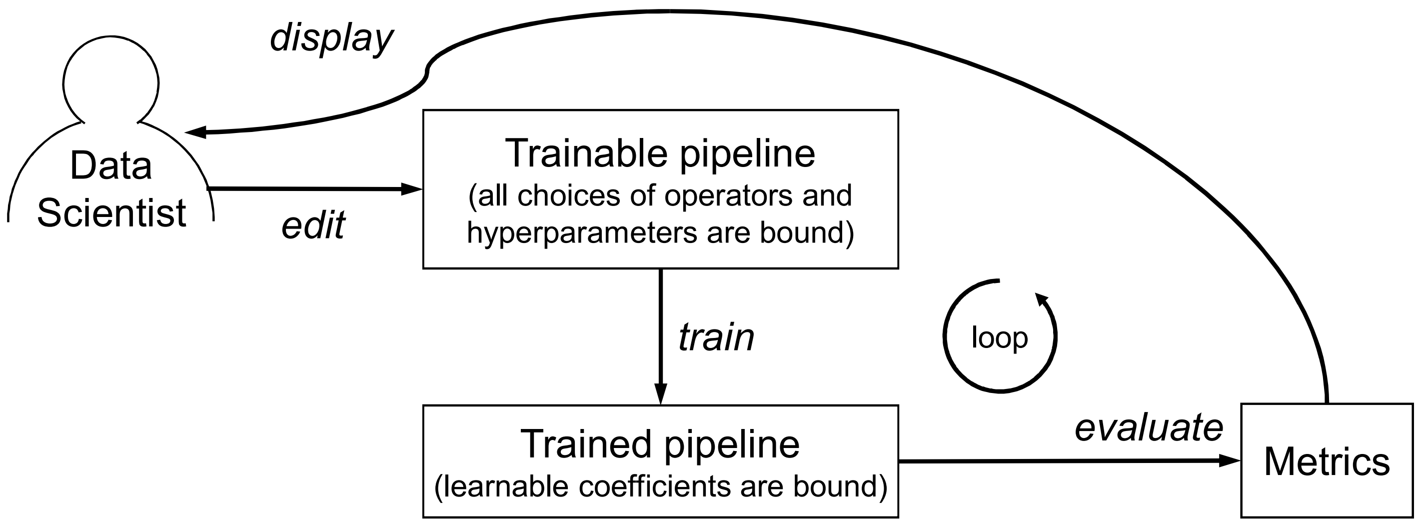
https://github.com/ibm/lale

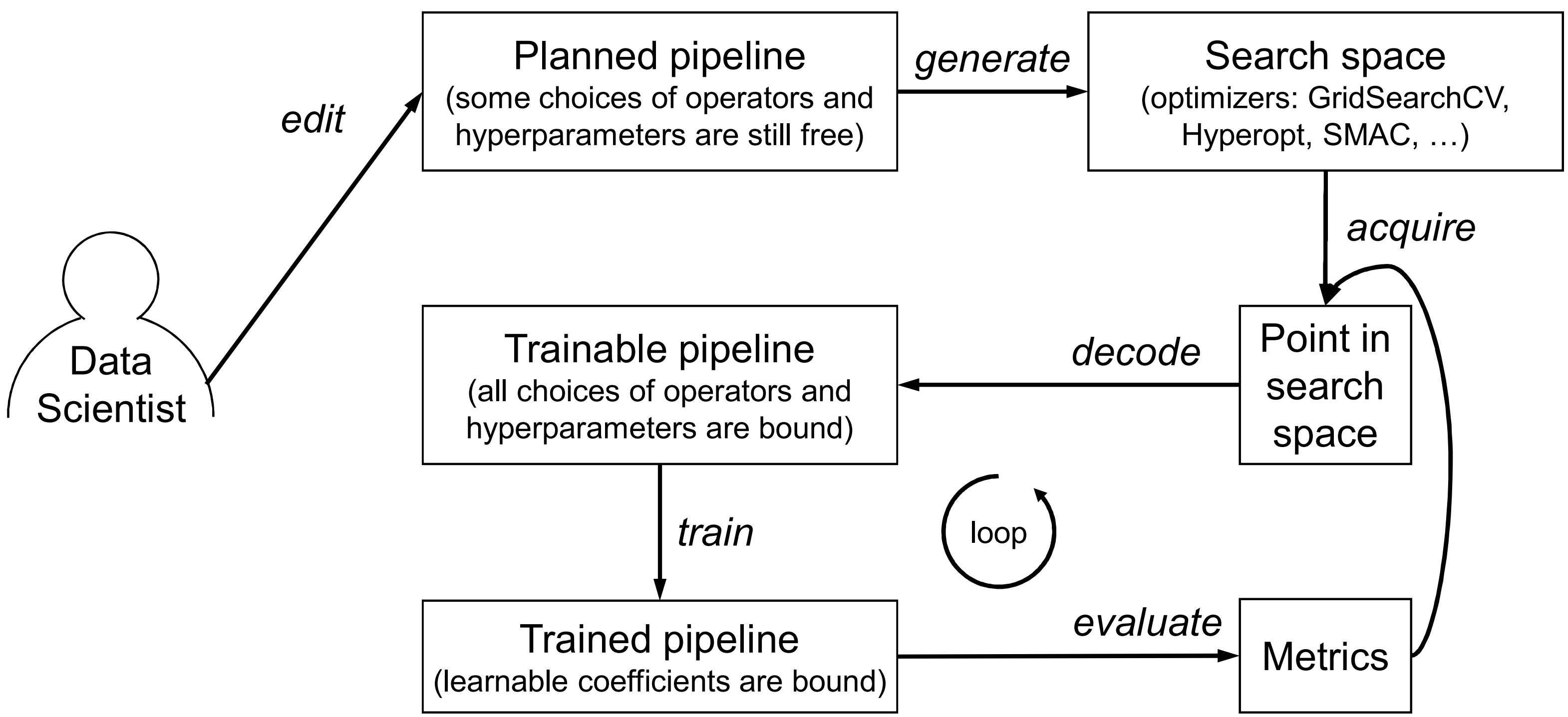
Manual Machine Learning



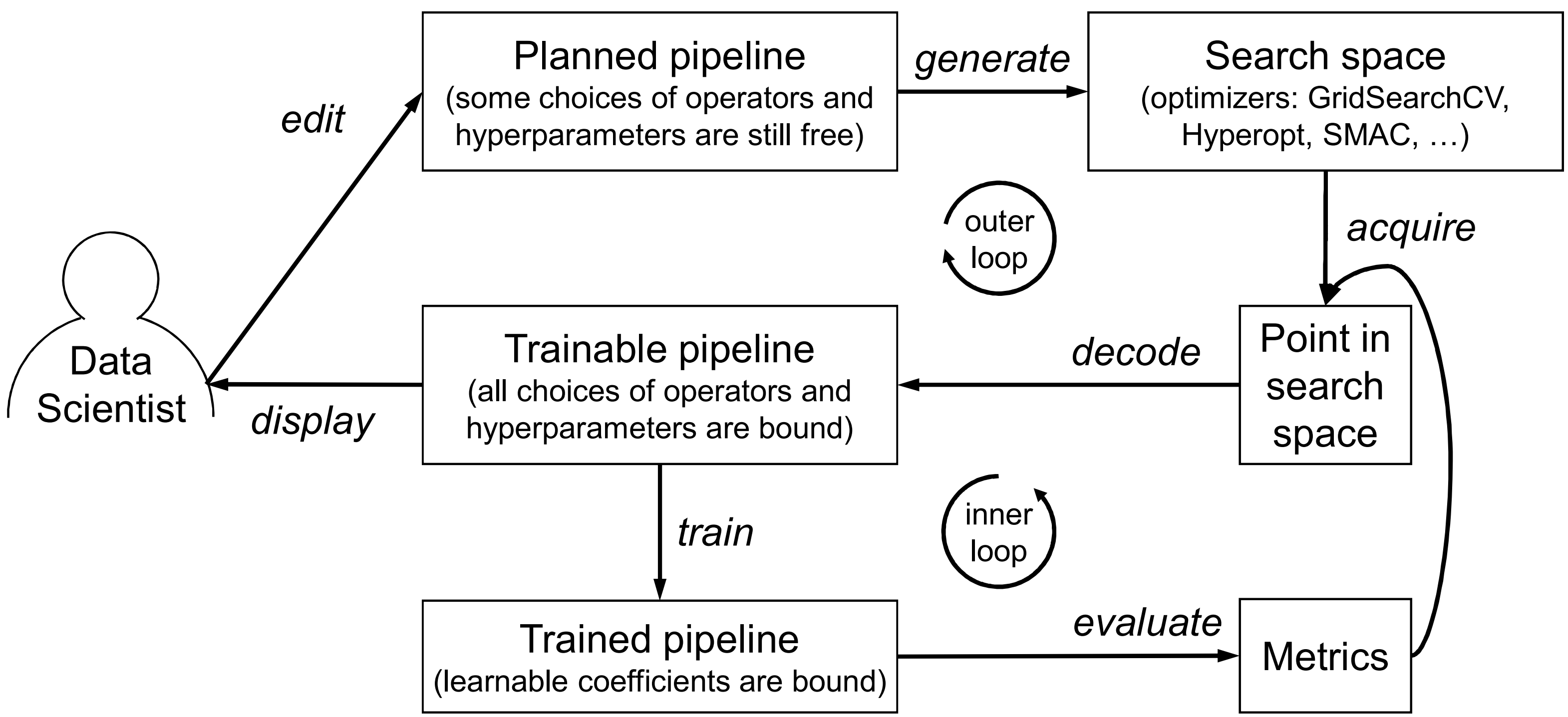
Iterated Manual Machine Learning



AutoML: Automated Machine Learning



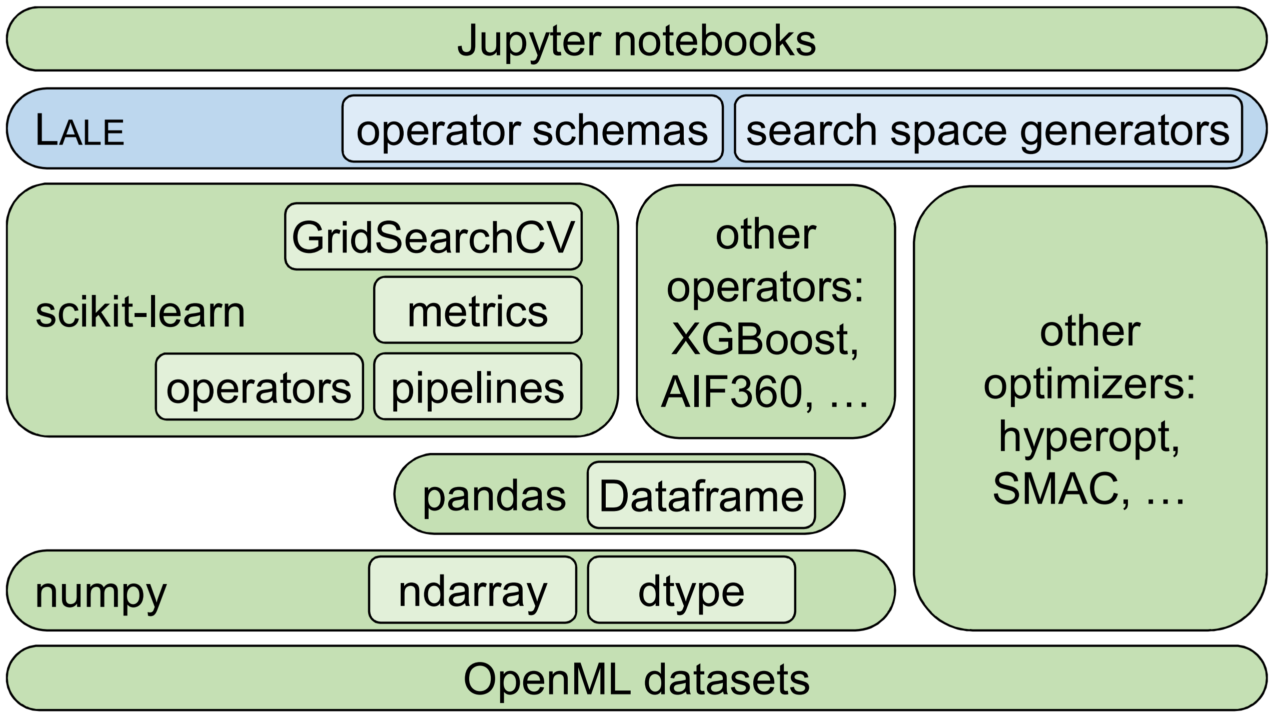
Iterated AutoML



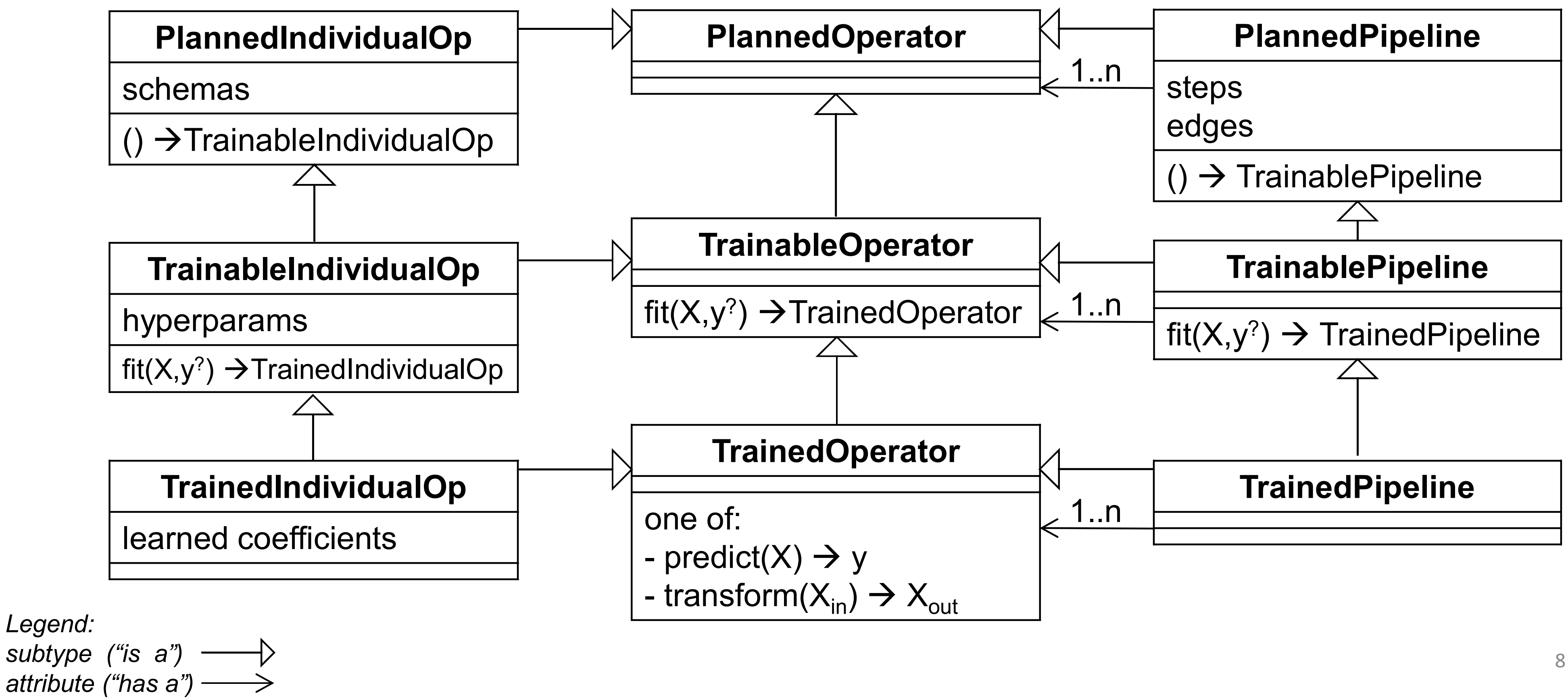
Problem Statement

- Library for semi-automated data science
- Easy-to-use automation
- Consistency of manual vs. automated experience
- Consistency across AutoML optimizers
- Display and iterative refinement
- Expert-level control

Open-Source AutoML Technologies



Operators, Pipelines, and Lifecycle



Example

- Dataset
- Manual machine learning
- Hyperparameter tuning
- Inspecting AutoML results
- Algorithm selection

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Covertype Dataset

In [4]:

```
import pandas as pd
pd.set_option('display.max_columns', None)
pd.concat([pd.DataFrame({'y': train_y}, index=train_X.index),
           train_X], axis=1).tail(10)
```

Out[4]:

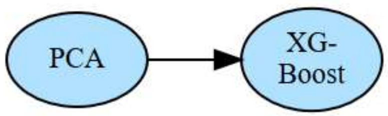
	y	Elevation	Aspect	Slope	Horizontal_Distance_To_Hydrology	Vertical_Distance_To_Hydrology	Horizontal_Distance_To_Roadways	Hillshade_9am	Hil
325384	2	3064.0	86.0	25.0	702.0	259.0	721.0	247.0	
442177	1	3277.0	31.0	15.0	454.0	70.0	1570.0	215.0	
185316	2	3138.0	257.0	14.0	228.0	30.0	5649.0	185.0	
189541	3	2317.0	150.0	8.0	150.0	42.0	644.0	231.0	
428374	2	2970.0	47.0	25.0	319.0	100.0	1919.0	220.0	
234638	1	3278.0	335.0	5.0	360.0	35.0	5763.0	209.0	
172207	1	3175.0	343.0	17.0	162.0	3.0	4395.0	183.0	
240801	1	3355.0	346.0	16.0	180.0	6.0	1922.0	188.0	
435277	1	3154.0	316.0	26.0	339.0	122.0	2688.0	143.0	
297100	7	3344.0	313.0	20.0	0.0	0.0	4317.0	163.0	

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Manual Machine Learning

In [5]:
```
from sklearn.decomposition import PCA
from xgboost import XGBClassifier as XGBoost
lale.wrap_imported_operators()
```

In [6]:
```
manual_trainable = PCA(n_components=6) >> XGBoost(n_estimators=3)
manual_trainable.visualize()
```



In [7]:
```
%%time
manual_trained = manual_trainable.fit(train_X, train_y)
```

```
CPU times: user 2.34 s, sys: 1.2 s, total: 3.55 s
Wall time: 2.05 s
```

In [8]:
```
import sklearn.metrics
manual_y = manual_trained.predict(test_X)
print(f'accuracy {sklearn.metrics.accuracy_score(test_y, manual_y):.1%}')
```

```
accuracy 64.5%
```

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Hyperparameter Tuning

In [9]:
```
XGBoost.hyperparam_schema('n_estimators')
```

Out[9]:
```
{'description': 'Number of trees to fit.',
 'type': 'integer',
 'default': 100,
 'minimumForOptimizer': 10,
 'maximumForOptimizer': 1500}
```

In [10]:
```
print(PCA.documentation_url())
```

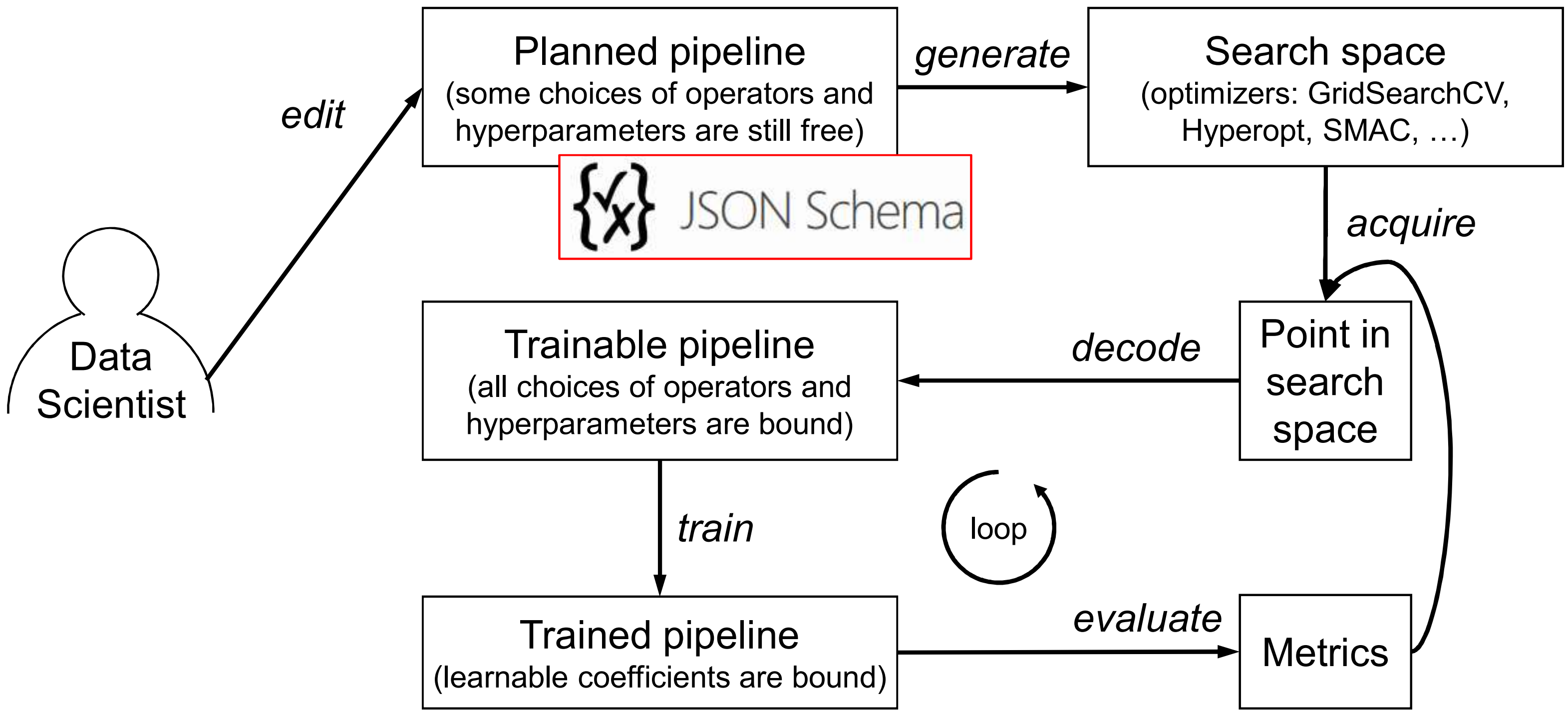
```
https://lale.readthedocs.io/en/latest/modules/lale.lib.sklearn.pca.html
```

In [11]:
```
from lale.lib.lale import Hyperopt
import lale.schemas as schemas

CustomPCA = PCA.customize_schema(n_components=schemas.Int(min=2, max=54))
CustomXGBoost = XGBoost.customize_schema(n_estimators=schemas.Int(min=1, max=10))

hpo_planned = CustomPCA >> CustomXGBoost
hpo_trainable = Hyperopt(estimator=hpo_planned, max_evals=10, cv=3)
```

In [12]:
```
%%time
hpo_trained = hpo_trainable.fit(train_X, train_y)
```

```
100%|██████████| 10/10 [01:20<00:00,  6.64s/trial, best loss: -0.7885106540569516]
CPU times: user 1min 50s, sys: 22.2 s, total: 2min 12s
Wall time: 1min 28s
```

Types as Search Spaces



https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Inspecting AutoML Results

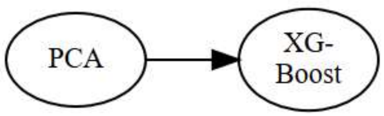
In [13]:

```
hpo_y = hpo_trained.predict(test_X)
print(f'accuracy {sklearn.metrics.accuracy_score(test_y, hpo_y):.1%}')
```

```
accuracy 80.1%
```

In [14]:

```
hpo_trained.get_pipeline().visualize()
```



In [15]:

```
hpo_trained.get_pipeline().pretty_print(ipython_display=True)
```

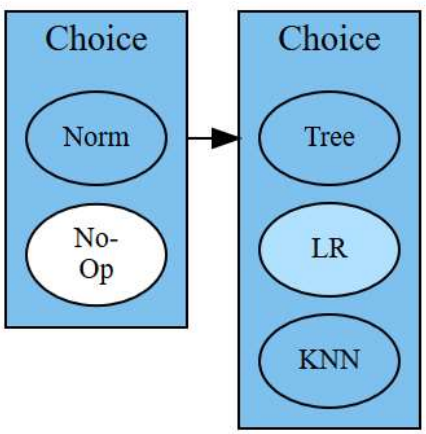
```
from lale.lib.sklearn import PCA
from lale.lib.xgboost.xgb_classifier import XGBoost
import lale
lale.wrap_imported_operators()

pca = PCA(n_components=39, svd_solver='full')
xg_boost = XGBoost(colsample_bylevel=0.6016063807304212, colsample_bytree=0.7763972782064467, learning_rate=0.16389357351003786, max_depth=10, min_child_weight=5, n_estimators=5, reg_alpha=0.10485915855270356, reg_lambda=0.9268502695024392, subsample=0.4503841871781402)
pipeline = pca >> xg_boost
```

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Algorithm Selection

In [19]:

```
from sklearn.preprocessing import Normalizer as Norm
from sklearn.linear_model import LogisticRegression as LR
from sklearn.tree import DecisionTreeClassifier as Tree
from sklearn.neighbors import KNeighborsClassifier as KNN
from lale.lib.lale import NoOp
lale.wrap_imported_operators()

KNN = KNN.customize_schema(n_neighbors=schemas.Int(min=1, max=10))
transp_planned = (Norm | NoOp) >> (Tree | LR(dual=True) | KNN)
transp_planned.visualize()
```



https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0327-lale.ipynb

Example: Combined Algorithm Selection and Hyperparameter Tuning

In [20]:

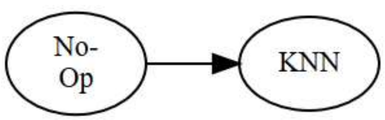
```
%%time
transp_trained = transp_planned.auto_configure(
    train_X, train_y, optimizer=Hyperopt, cv=3, max_evals=3)
```

```
100%|██████████| 3/3 [01:48<00:00, 32.59s/trial, best loss: -0.8376392446578157]
CPU times: user 1min 50s, sys: 1.12 s, total: 1min 51s
Wall time: 1min 49s
```

In [21]:

```
transp_trained.pretty_print(ipython_display=True, show_imports=False)
transp_trained.visualize()
```

```
knn = KNN(algorithm='ball_tree', metric='manhattan', n_neighbors=9)
pipeline = NoOp() >> knn
```



In [22]:

```
%%time
transp_y = transp_trained.predict(test_X)
print(f'accuracy {sklearn.metrics.accuracy_score(test_y, transp_y):.1%}')
```

```
accuracy 86.6%
CPU times: user 50.6 s, sys: 15.6 ms, total: 50.6 s
Wall time: 50.7 s
```

Expert-Level Control

- Custom metrics
- Non-linear pipelines
- Higher-order operators
- Adding new operators

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/demo_aif360.ipynb

Custom Metrics

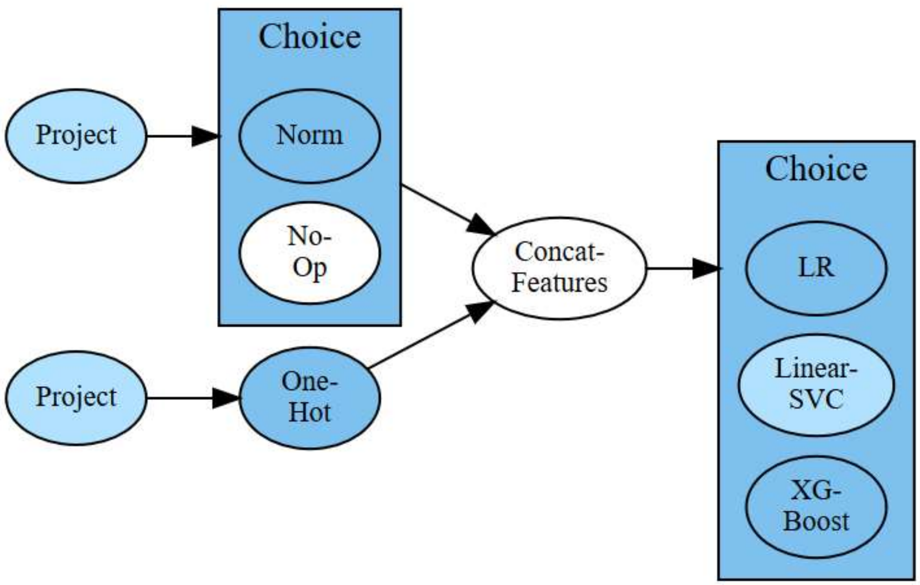
```
def fairness_scorer(pipeline, X, y):
    from sklearn.metrics import accuracy_score
    from aif360.datasets import BinaryLabelDataset
    predictions = pipeline.predict(X)
    accuracy = accuracy_score(y, predictions)
    df = pd.concat([X, y], axis=1)
    dataset_pred = BinaryLabelDataset(favorable_label=1., unfavorable_label=2.,
                                      protected_attribute_names=['sex', 'age'],
                                      df=df, label_names=['credit'])
    fairness_metrics = aif360.metrics.BinaryLabelDatasetMetric(
        dataset_pred, unpr_groups, priv_groups)
    disparate_impact = fairness_metrics.disparate_impact()
    #Hyperopt minimizes (best_score - score_returned_by_scorer), choosing the values below based on that.
    if disparate_impact < 0.9 or 1.1 < disparate_impact:
        return -99
    else:
        return accuracy
```

```
trained_fairer = planned_fairer.auto_configure(
    train_X, train_y, optimizer = Hyperopt, cv=3, max_evals=25, scoring=fairness_scorer, best_score=1.0)
```

https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/talk_2020-0302-lale.ipynb

Non-Linear Pipelines

```
project_nums = Project(columns={'type': 'number'})
project_cats = Project(columns={'type': 'string'})
planned_pipeline = (
        (project_nums >> (Norm | NoOp) & project_cats >> OneHot)
    >> ConcatFeatures
    >> (LR | LinearSVC(dual=False)| XGBoost))
planned_pipeline.visualize()
```



Pipeline Combinators

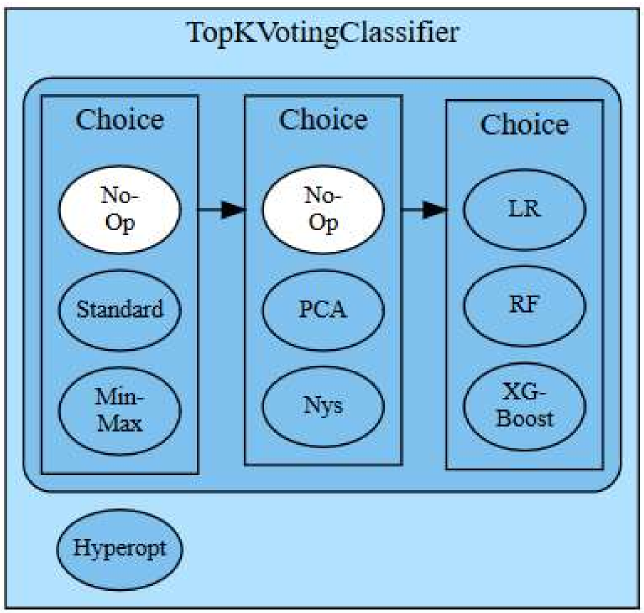
LALE features	Name	Description	Scikit-learn features
`>>` or `make_pipeline`	pipe	feed to next	`make_pipeline`
`&` or `make_union`	and	run both	`make_union` or `ColumnTransformer`
`|` or `make_choice`	or	choose one	N/A (specific to given Auto-ML tool)

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

Higher-Order Operators (1/2)

In [4]:

```
planned_pipeline = (NoOp | Standard | MinMax) >> (NoOp | PCA | Nys) >> (LR | RF | XGBoost)
ensemble = TopKVotingClassifier(
    estimator=planned_pipeline, k=3, optimizer=Hyperopt,
    args_to_optimizer={'max_evals':25, 'scoring':'accuracy'})
ensemble.visualize()
```



In [5]:

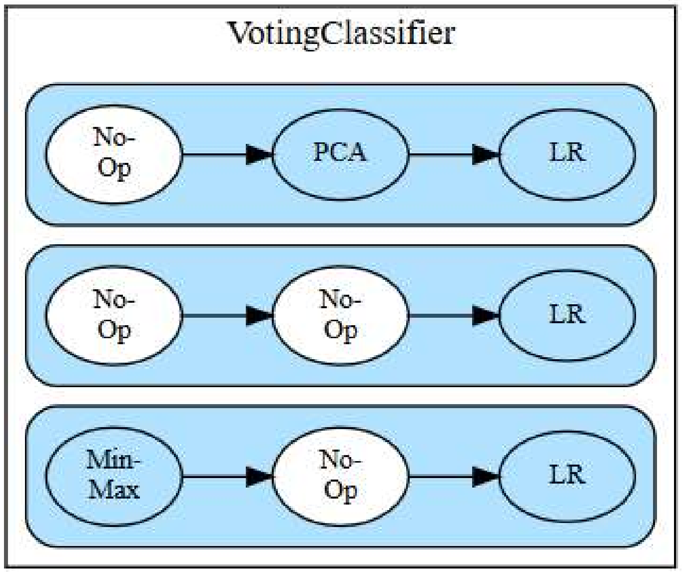
```
trained_ensemble = ensemble.fit(train_X, train_y)
```

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

Higher-Order Operators (2/2)

In [8]:

```
best_pipeline = trained_ensemble.get_pipeline()
best_pipeline.visualize()
```



Type-Driven Automated Learning

- Types as search spaces
  - E.g., continuous hyperparameter range
  - E.g., categorical hyperparameter enum
- Types as documentation
  - E.g., lale.readthedocs.io/en/latest/modules/lale.lib.sklearn.pca.html
- Types for feature engineering
  - E.g., Project(columns={'type': 'string’})
- Types for error checking
  - E.g., datasets, hyperparameters, constraints

Conclusion

- Library for semi-automated data science
  - https://github.com/ibm/lale
- Suggested actions:
  - Try it out and send us feedback
  - Contribute new individual operators:
    https://nbviewer.jupyter.org/github/IBM/lale/blob/master/examples/docs_new_operators.ipynb
  - Do original research (AutoML optimizers, AI fairness, fast AutoML, …)