How to use scikit-learn to solve machine learning problems

AutoML Hackathon

April 2015

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Datageek, contributor to scikit-learn, works with Python / Java / Clojure / Pig, interested in Machine Learning, NLProc, {Big|Linked|Open} Data and braaains!

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Outline

- Machine Learning refresher
- scikit-learn
- Demo: interactive predictive modeling on Census Data with IPython notebook / pandas / scikit-learn
- Combining models with Pipeline and parameter search

Predictive modeling ~= machine learning

- Make predictions of outcome on new data
- Extract the structure of historical data
- Statistical tools to summarize the training data into a executable predictive model
- Alternative to hard-coded rules written by experts

type (category)	# rooms (int)	surface (float m2)	public trans (boolean)
Apartment	3	50	TRUE
House	5	254	FALSE
Duplex	4	68	TRUE
Apartment	2	32	TRUE

type (category)	# rooms (int)	surface (float m2)	public trans (boolean)	sold (float k€)
Apartment	3	50	TRUE	450
House	5	254	FALSE	430
Duplex	4	68	TRUE	712
Apartment	2	32	TRUE	234

features

target

type (category)	# rooms (int)	surface (float m2)	public trans (boolean)	sold (float k€)
Apartment	3	50	TRUE	450
House	5	254	FALSE	430
Duplex	4	68	TRUE	712
Apartment	2	32	TRUE	234

samples (train)

features

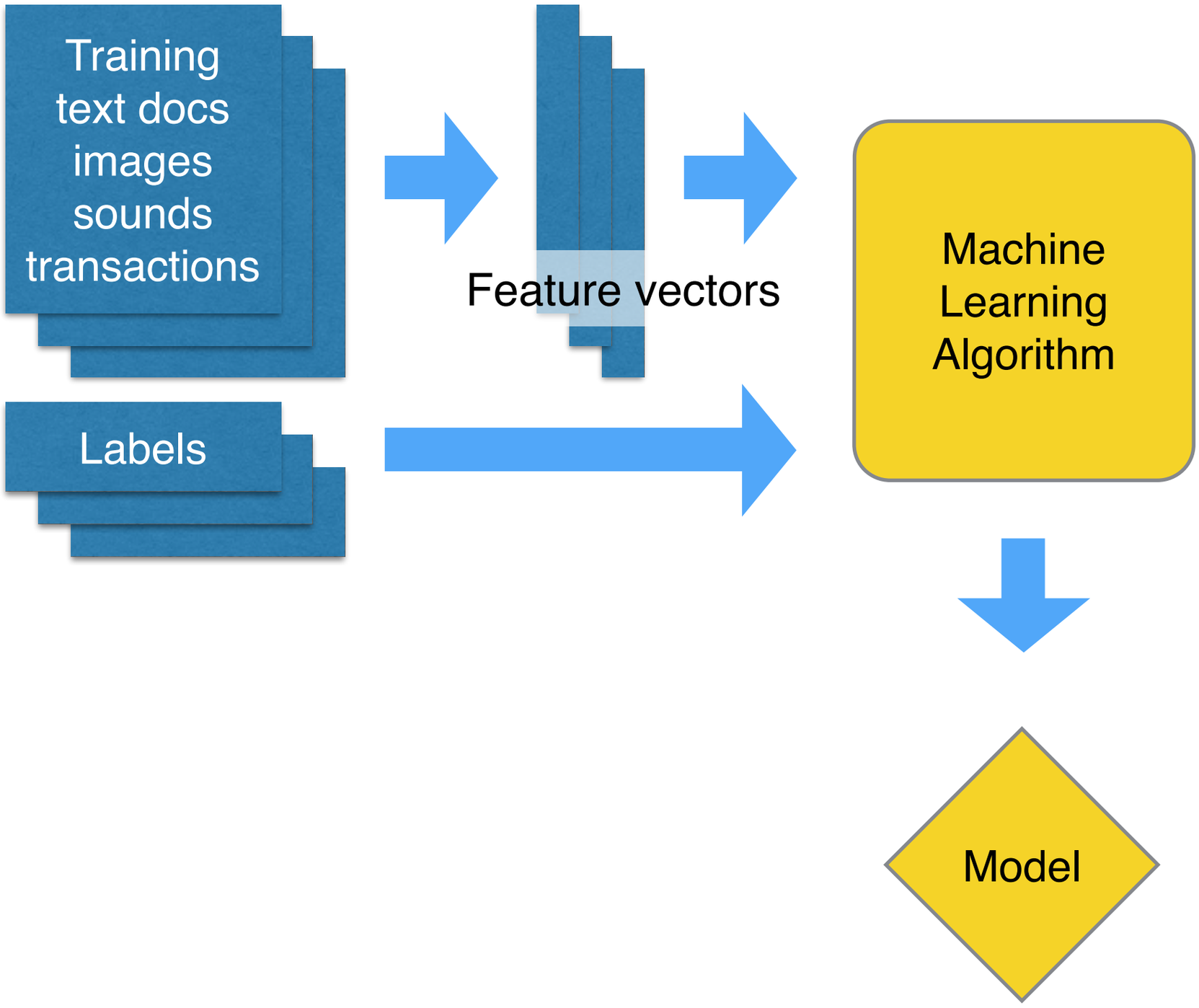
target

samples (train)

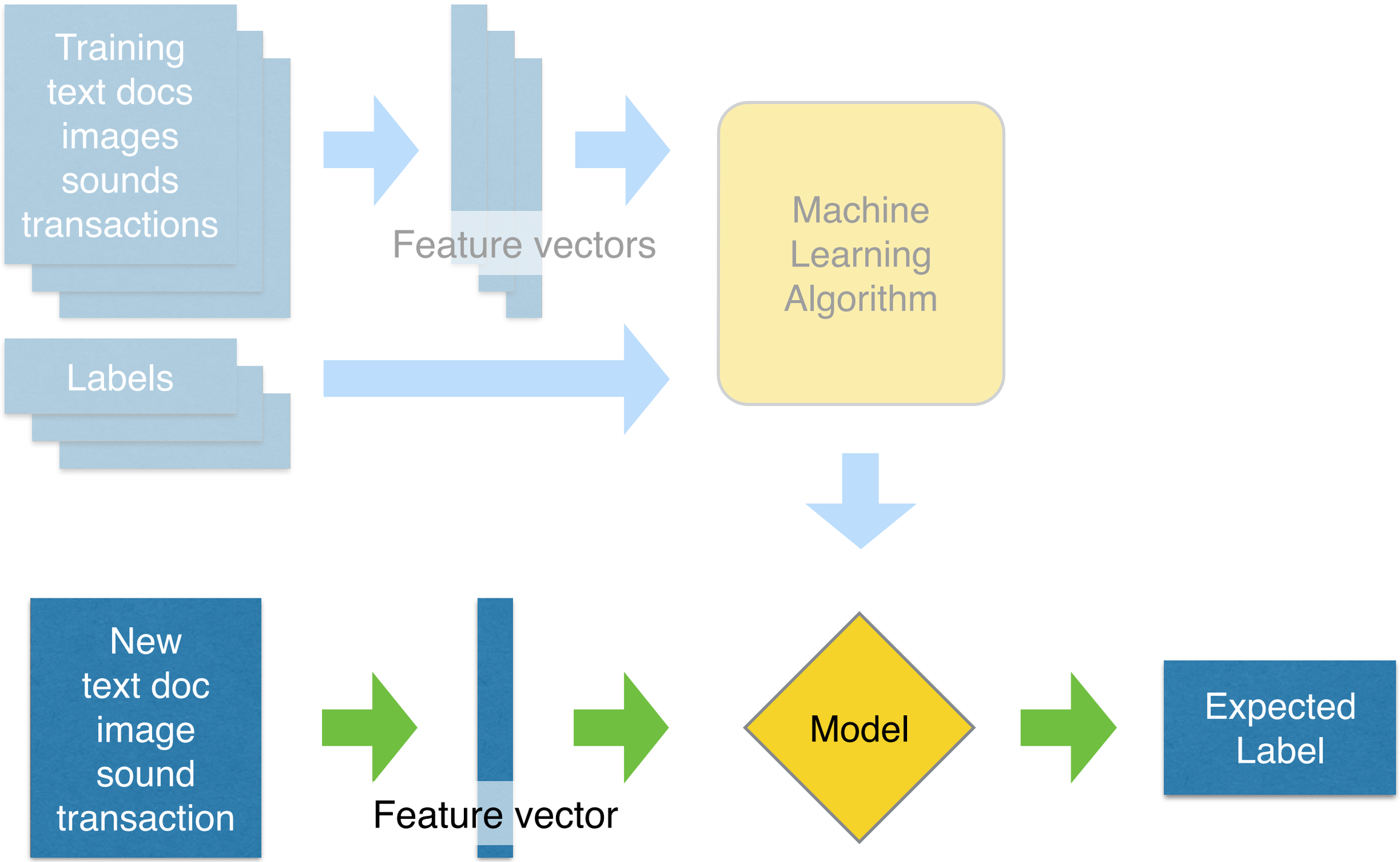
type (category)	# rooms (int)	surface (float m2)	public trans (boolean)	sold (float k€)
Apartment	3	50	TRUE	450
House	5	254	FALSE	430
Duplex	4	68	TRUE	712
Apartment	2	32	TRUE	234

samples (test)

Apartment	2	33	TRUE	?
House	4	210	TRUE	?



Predictive Modeling Data Flow



Predictive Modeling Data Flow

Predictive modeling in the wild

Virality and readers engagement

Fraud detection

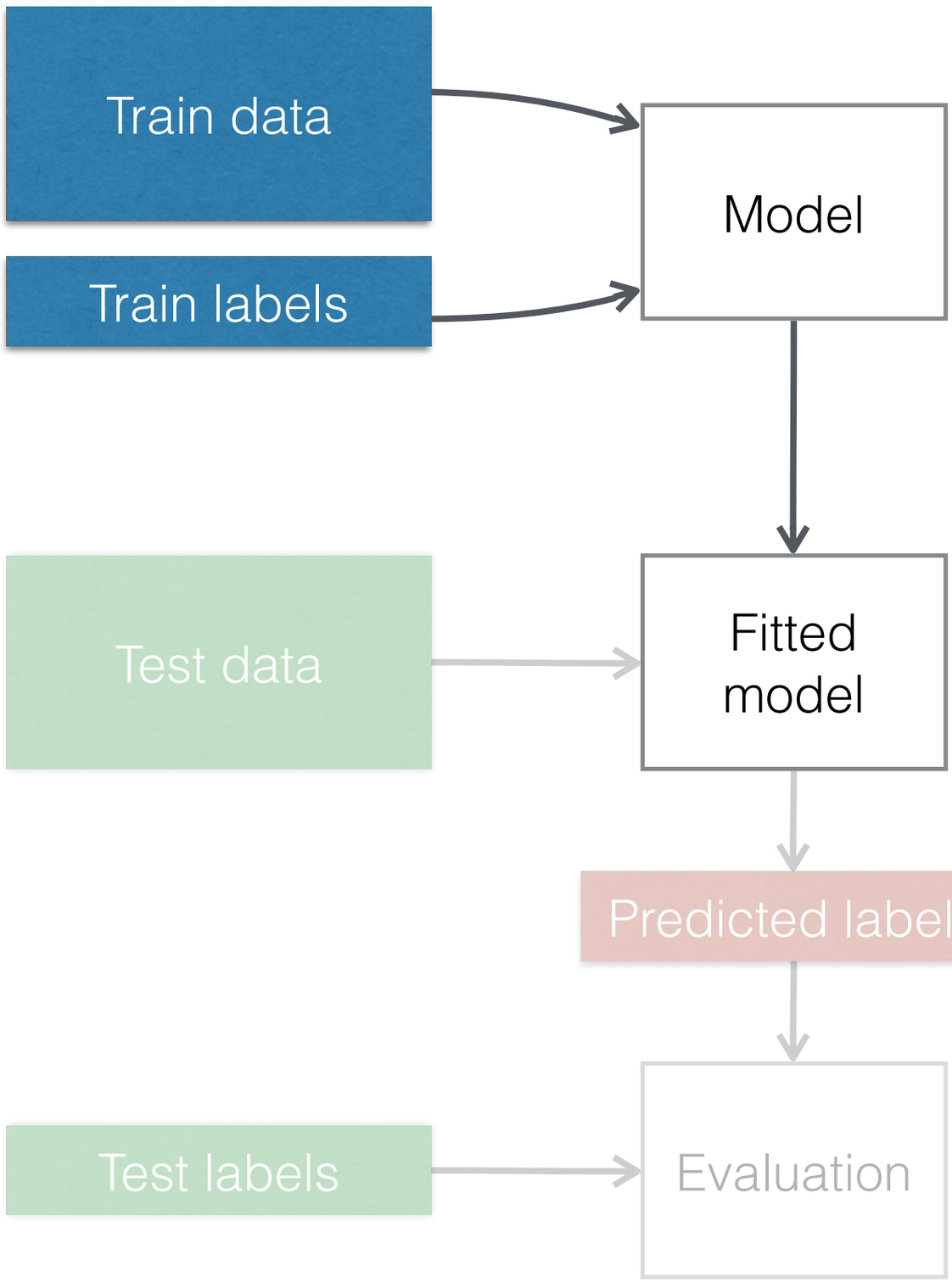
Personalized radios

Inventory forecasting & trends detection

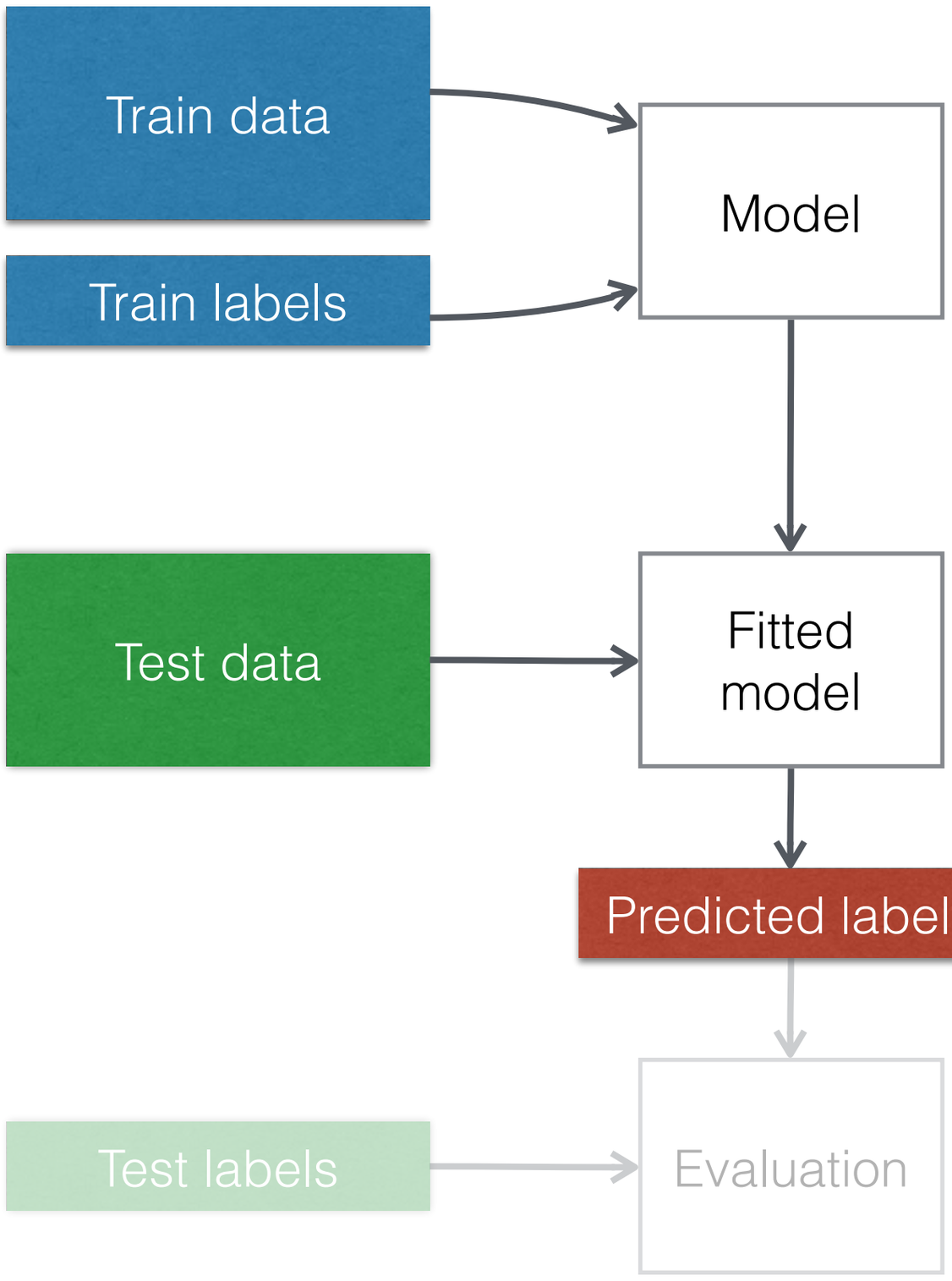
Predictive maintenance

Personality matching

- Library of Machine Learning algorithms
- Focus on established methods (e.g. ESL-II)
- Open Source (BSD)
- Simple **`fit`** / **`predict`** / **`transform`** API
- Python / NumPy / SciPy / Cython
- Model Assessment, Selection & Ensembles

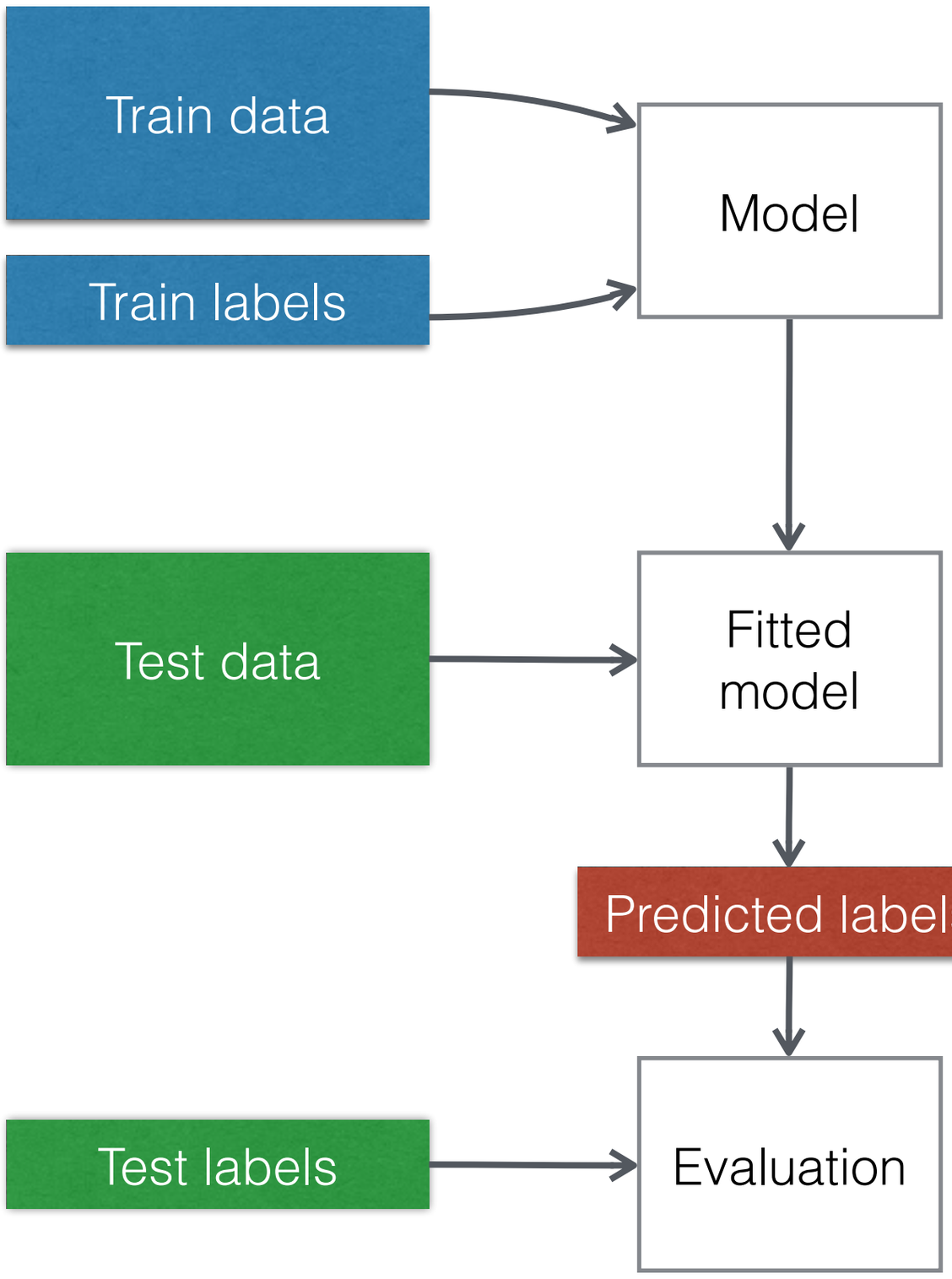



```
model = ModelClass(**hyperparams)
model.fit(X_train, y_train)
```




```
model = ModelClass(**hyperparams)
model.fit(X_train, y_train)
```

```
y_pred = model.predict(X_test)
```




```
model = ModelClass(**hyperparams)
model.fit(X_train, y_train)
```

```
y_pred = model.predict(X_test)
```

```
accuracy_score(y_test, y_pred)
```

Support Vector Machine

```
from sklearn.svm import SVC

model = SVC(kernel="rbf", C=1.0, gamma=1e-4)
model.fit(X_train, y_train)


y_predicted = model.predict(X_test)

from sklearn.metrics import f1_score
f1_score(y_test, y_predicted)
```

Linear Classifier

```
from sklearn.linear_model import SGDClassifier

model = SGDClassifier(alpha=1e-4,
                      penalty="elasticnet")
model.fit(X_train, y_train)


y_predicted = model.predict(X_test)

from sklearn.metrics import f1_score
f1_score(y_test, y_predicted)
```

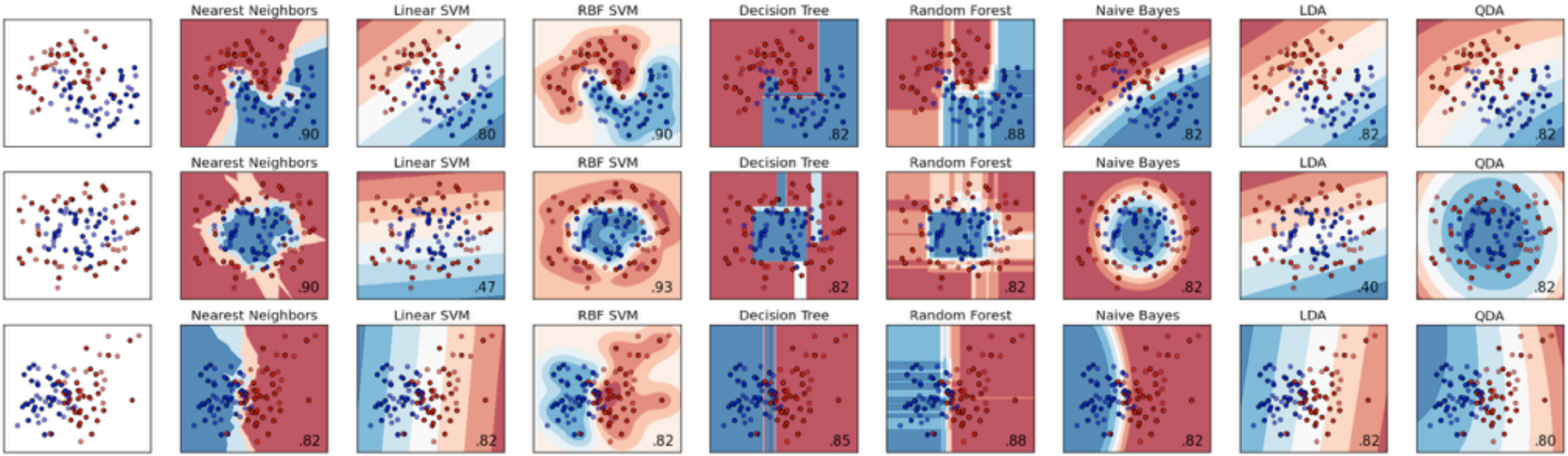
Random Forests

```
from sklearn.ensemble import RandomForestClassifier

model = RandomForestClassifier(n_estimators=200)
model.fit(X_train, y_train)


y_predicted = model.predict(X_test)

from sklearn.metrics import f1_score
f1_score(y_test, y_predicted)
```


Nearest Neighbors
Linear SVM
RBF SVM
Decision Tree
Random Forest
Naive Bayes
LDA
QDA
.90
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Nearest Neighbors
Linear SVM
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Decision Tree
Random Forest
Naive Bayes
LDA
QDA
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Nearest Neighbors
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Naive Bayes
LDA
QDA
.82
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scikit-learn: machine learning in Python — scikit-learn 0.14 documentation

scikit-learn: machine learning i...

scikit-learn.org/stable/

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scikit learn

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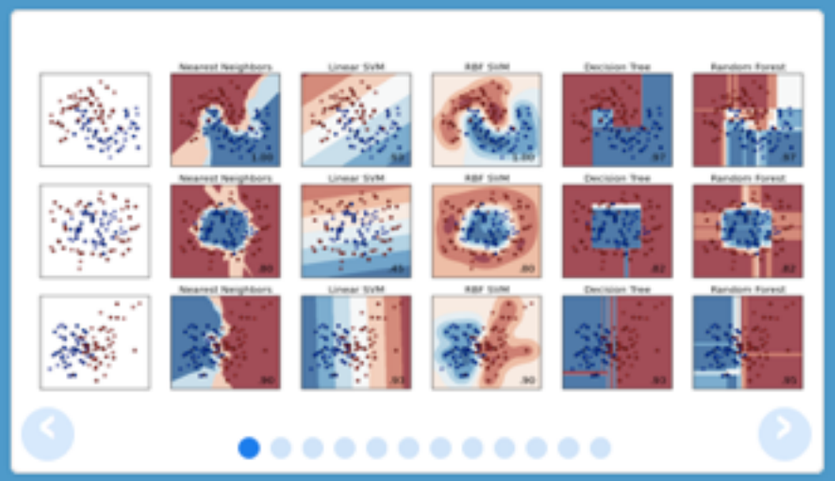

scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying to which set of categories a new observation belong to.

Applications: Spam detection, Image recognition.
Algorithms: *SVM*, *nearest neighbors*, *random forest*, ... — *Examples*

Regression

Predicting a continuous value for a new example.

Applications: Drug response, Stock prices.
Algorithms: *SVR*, *ridge regression*, *Lasso*, ... — *Examples*

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: *k-Means*, *spectral clustering*, *mean-shift*, ... — *Examples*

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: *PCA*, *Isomap*, *non-negative matrix factorization*. — *Examples*

Model selection

Comparing, validating and choosing parameters and models.

Goal: Improved accuracy via parameter tuning
Modules: *grid search*, *cross validation*, *metrics*. — *Examples*

Preprocessing

Feature extraction and normalization.

Application: Transforming input data such as text for use with machine learning algorithms.
Modules: *preprocessing*, *feature extraction*. — *Examples*

Demo time!

http://nbviewer.ipython.org/github/ogrisel/notebooks/blob/master/sklearn_demos/Income%20classification.ipynb

https://github.com/ogrisel/notebooks

Combining Models

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import RandomizedPCA
from sklearn.svm import SVC

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)

pca = RandomizedPCA(n_components=10)
X_train_pca = pca.fit_transform(X_train_scaled)

svm = SVC(C=0.1, gamma=1e-3)
svm.fit(X_train_pca, y_train)
```

Pipeline

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import RandomizedPCA
from sklearn.svm import SVC
from sklearn.pipeline import make_pipeline
```

```
pipeline = make_pipeline(
    StandardScaler(),
    RandomizedPCA(n_components=10),
    SVC(C=0.1, gamma=1e-3),
)

pipeline.fit(X_train, y_train)
```

Scoring manually stacked models

```
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)

pca = RandomizedPCA(n_components=10)
X_train_pca = pca.fit_transform(X_train_scaled)

svm = SVC(C=0.1, gamma=1e-3)
svm.fit(X_train_pca, y_train)

X_test_scaled = scaler.transform(X_test)
X_test_pca = pca.transform(X_test_scaled)
y_pred = svm.predict(X_test_pca)
accuracy_score(y_test, y_pred)
```

Scoring a pipeline

```
pipeline = make_pipeline(
    RandomizedPCA(n_components=10),
    SVC(C=0.1, gamma=1e-3),
)
pipeline.fit(X_train, y_train)


y_pred = pipeline.predict(X_test)
accuracy_score(y_test, y_pred)
```

Parameter search

```
import numpy as np
from sklearn.grid_search import RandomizedSearchCV

params = {
    'randomizedpca__n_components': [5, 10, 20],
    'svc__C': np.logspace(-3, 3, 7),
    'svc__gamma': np.logspace(-6, 0, 7),
}
search = RandomizedSearchCV(pipeline, params,
                            n_iter=30, cv=5)
search.fit(X_train, y_train)
# search.best_params_, search.grid_scores_
```

Thank you!

- http://scikit-learn.org

- https://github.com/scikit-learn/scikit-learn

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